Spectral Theory of the Atomic Dirac Operator in the No-Pair Formalism

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Das schönste Glück des denkenden Menschen ist,
das Erforschliche erforscht zu haben
und das Unerforschliche ruhig zu verehren.

(Goethe)

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Zusammenfassung

Die auf Dirac zurückgehende relativistische Beschreibung der Bewegung von Teilchen in einem Zentralfeld führt zu der Besonderheit, daß es neben den Zuständen mit positiver Energie auch solche mit beliebig kleiner (negativer) Energie gibt, die den entsprechenden Antiteilchen zugeordnet werden. Obwohl man in der Physik voraussetzt, daß im Grundzustand alle Niveaus mit negativer Energie besetzt sind, treten Probleme immer dann auf, wenn keine exakte Lösung der Dirac-Gleichung angegeben werden kann. Hat der Energieerwartungswert keine untere Schranke, so können zur Bestimmung der Energiezustände die üblichen Variationsverfahren, die auf eine Minimierung der Energie abzielen, nicht angewandt werden. Es sind entweder sogenannte Minimax-Prozeduren vonnöten, oder man muß auf andere Methoden ausweichen.

Ein von Foldy und Wouthuysen für freie Teilchen und später von Douglas und Kroll für Teilchen im Zentralfeld vorgestellter Lösungsversuch des Problems des negativen Energiekontinuums besteht darin, mit Hilfe einer unitären Transformation die positiven und negativen Energiezustände zu entkoppeln. Wenn die Erzeugung von Teilchen-Antiteilchen-Paaren ausgeschlossen werden kann (z.B. in der Spektroskopie von Atomen), so kann man sich durch diese Methode auf die Berücksichtigung positiver Energiezustände beschränken. Bei Anwesenheit eines Zentralpotentials gelingt die Entkopplung nicht exakt, es ist jedoch möglich, für nicht zu starke (sogenannte unterkritische) Zentralfelder eine störungstheoretische Entwicklung nach der Potentialstärke vorzunehmen.

Von Hess und Mitarbeitern wurde der aus dieser Transformation resultierende Operator in quantenchemischen Rechnungen zur Struktur der Atome eingesetzt. Aus mathematischer Sicht erhebt sich jedoch die Frage, ob der neue Operator wirklich nur positive Energiezustände besitzt, ob die störungstheoretische Entwicklung konvergiert, und vor allem, wie groß die Potentialstärke maximal sein darf, damit diese Eigenschaften vorliegen.

Während der nach Brown und Ravenhall benannte, die Potentialstärke bis maximal erster Ordnung enthaltende Operator ausführlich mathematisch analysiert worden ist, ist von dem von Jansen und Hess eingeführten Operator, der zusätzlich den quadratischen Term in der Potentialstärke enthält, bisher nur seine Beschränktheit nach unten, sowie seine Positivität im fiktiven Fall eines einzigen, masselosen Teilchens gezeigt worden. Dabei stimmt im untersuchten Fall des reinen Coulombpotentials die maximal zulässige Potentialstärke (die durch die Ladung des Zentralkerns festgelegt ist) fast genau mit derjenigen überein, die man aus einer exakten quantenmechanischen Rechnung für das Nullwerden der Grundzustandsenergie erhält.

In der vorliegenden Arbeit wird ein unitäres Transformationsschema vorgestellt, das in der mathematischen Festkörperphysik zur Untersuchung der Teilchenbewegung in beschränkten, periodischen Potentialen bereits erfolgreich angewandt worden ist. Dieses führt zu einer sehr einfachen Darstellung der transformierten Operatoren und ermöglicht somit eine mathematische Analyse auch im Fall mehrerer Teilchen.

Zunächst wird im Einteilchenfall die unitäre Äquivalenz des neuen Transformationsschemas zu der von Douglas und Kroll eingeführten Transformation gezeigt. Sodann wird die Formbeschränktheit und Positivität des Jansen-Hess-Operators für massebehaftete Teilchen untersucht und sein wesentliches Spektrum und Punktspektrum lokalisiert. Betreffs der Konvergenz der störungstheoretischen Entwicklung im hier untersuchten Fall des reinen Coulombfeldes kann nur die Dominanz

des Anteils erster Ordnung bezüglich des Anteils zweiter Ordnung in der Potentialstärke nachgewiesen werden. Im Rahmen des hier verwendeten Verfahrens ist eine generelle Aussage für die Terme höherer Ordnung nicht möglich. Für ein Zentralfeld mit leicht abgeschwächter Singularität läßt sich jedoch zeigen, daß die Terme höherer Ordnung von den Termen niedrigerer Ordnung kontrolliert werden und daß die Entwicklung konvergiert.

Die gleichen Untersuchungsmethoden werden sodann auf den Zweiteilchenfall angewandt, wobei zum ersten Mal auch die Zweiteilchenwechselwirkung bis inklusive zweiter Ordnung in der Kopplungskonstanten berücksichtigt wird. Auch hier läßt sich Formbeschränktheit, Dominanz der linearen über die quadratischen Potentialterme, sowie Positivität zeigen. Die im Rahmen der hier angewandten Abschätzungen sich ergebende kritische Potentialstärke für die Gültigkeit dieser Eigenschaften liegt leicht unterhalb derjenigen des Einteilchenfalls.

Für das Zweiteilchenspektrum kann gezeigt werden, daß das wesentliche Spektrum dasjenige zweier freier Teilchen umfaßt und sich nicht ändert, wenn man die Zweiteilchenwechselwirkung zweiter Ordnung wegläßt. Außerdem existieren keine Eigenwerte, wenn die Teilchenmasse zu null gesetzt wird.

Abschließend wird ein kurzer Ausblick auf den transformierten Operator zweiter Ordnung im allgemeinen Fall von N Teilchen gegeben. Dieser Operator kann explizit angegeben und seine Positivität bestimmt werden. Die sich dabei ergebende kritische Potentialstärke für ein neutrales Atom ist deutlich niedriger als im Einteilchenfall. Wenngleich die hier verwendeten Methoden keine optimale Schranke für die zulässige Potentialstärke liefern, ist dies doch ein Indiz dafür, daß man die Zweiteilchenpotentiale höherer Ordnung nicht, wie bislang üblich, vernachlässigen sollte.

Abstract

By means of a unitary transformation scheme borrowed from the study of quantum lattice systems, the Dirac operator of a one-electron ion is transformed into a pseudo-relativistic operator which easily allows for the elimination of the positron degrees of freedom. This operator is block-diagonal with respect to the projection onto the positive (respective negative) spectral subspace of the free Dirac operator, to a fixed order in the strength of the electron-nucleus Coulomb potential. It is demonstrated that this transformation scheme is unitarily equivalent to the one introduced by Douglas and Kroll, and that the pseudo-relativistic operators of (up to) first and second order in the potential strength agree with the Brown-Ravenhall and the Jansen-Hess operator, respectively. The transformation scheme is successively applied to two-electron and N-electron systems in a Coulomb central field, and it is shown that the transformation operators are well-defined and that the potential terms of the resulting pseudo-relativistic operators are relatively bounded with respect to the kinetic energy operator for subcritical potential strength. In the case of a modified Coulomb potential, $V = -\gamma x^{-1+\epsilon}, \quad 0 < \epsilon \ll 1,$ one can even prove subordinacy of the higher-order potential terms and thus convergence of the perturbation series.

The investigations of Evans, Perry and Siedentop and of Balinsky and Evans, concerning the single-particle Brown-Ravenhall operator are extended to the Jansen-Hess operator. It is shown that its essential spectrum is given by $[m, \infty)$ for potential strengths $\gamma < 1.006,$ that the singular continuous spectrum is empty and that for $\gamma < 0.29$, there are no embedded eigenvalues in $[m, \infty);$ also, that for massless particles, the spectrum is absolutely continuous. Whereas positivity of the massless Jansen-Hess operator was proved by Brummelhuis, Siedentop and Stockmeyer for $\gamma \leq 1.006$, we were in the massive case only able to show positivity for $\gamma \leq 0.83$. For the two-electron ion and N-electron atom, positivity is established for $\gamma \leq 0.82$ and $\gamma \leq 0.44$, respectively. The large reduction of the critical potential strength for the N-electron atom is attributed to the two-particle second-order potential terms in the pseudo-relativistic operator. Although our bounds on γ are not sharp, this is a challenge to the quantum chemists who are usually neglecting these terms.

Apart from positivity, also the relative boundedness of the second-order potential terms with respect to the first-order potential terms is investigated for the two-particle pseudo-relativistic operator, as well as its spectrum. It is found that the free-particle positive spectrum $[2m, \infty)$ is a subset of the essential spectrum of the full two-particle pseudo-relativistic operator (for $\gamma < 0.89$), and that the essential spectrum does not change when the two-particle second-order interaction terms are dropped (for $\gamma < 0.65$). Again, eigenvalues are absent in the massless case. This property holds for $\gamma < 0.98$.

Introduction

With the advent of relativistic quantum mechanics (Dirac 1928), the analysis of Dirac operators has played an important role in mathematical physics. Relativity covers two aspects, particles moving at high velocity (close to the velocity c of light) or being exposed to very strong potentials. For a single particle with mass m and spin $\frac{1}{2}$ in an electric potential V the Dirac operator reads (in relativistic units $\hbar = c = 1$)

$$H \;=\; D_0 \,+\, V \quad = \,-i\,\boldsymbol{\alpha}\,\frac{\partial}{\partial \mathbf{x}} \,+\, \beta m \,+\, V$$

where D_0 is the Dirac operator of a free particle (i.e. its kinetic energy operator), and $\beta,\ \alpha_i,\ i = 1,2,3$ are the Dirac matrices in $\mathbb{C}^{4,4}$ (Rose 1961)

$$\alpha_i \;=\; \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \qquad \beta \;=\; \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

$$\sigma_1 \;=\; \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 \;=\; \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 \;=\; \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

with σ_i the Pauli matrices and I the 2×2 unit matrix. D_0 is defined in the Hilbert space $\mathcal{H} := L_2(\mathbb{R}^3) \times \mathbb{C}^4$. $\mathcal{H}$ is equipped with the scalar product $(\varphi, \psi) := \int_{\mathbb{R}^3} \overline{\varphi(\mathbf{x})}\psi(\mathbf{x})\, d\mathbf{x}$ where $\overline{\varphi}\psi := \sum_{i=1}^{4} \overline{\varphi}_i \psi_i$, the sum running over the 4 components φ_i, ψ_i of the spinors φ and ψ.

D_0 is self-adjoint on its domain $\mathcal{D}(D_0) \subset \mathcal{H}$. The potential V is a multiplication operator in coordinate space. In order that the sum $D_0 + V$ is also a self-adjoint operator on $\mathcal{D}(D_0)$, the potential must be controlled by the kinetic energy, i.e., V has to be D_0-bounded,

$$\|V\,\varphi\| \;\leq\; c\,\|D_0\,\varphi\| \;+\; C\,\|\varphi\|$$

with $c < 1$ and $C \in \mathbb{R}$ (Kato 1966, p.287).

Below we will define H in terms of its quadratic form, subject to the relative form boundedness of V with respect to $|D_0|$,

$$|(\varphi, V\,\varphi)| \;\leq\; c\,(\varphi, |D_0|\,\varphi) \;+\; C\,(\varphi, \varphi)$$

with $c < 1$ and $|D_0| := (D_0^2)^{1/2}$. We will take the spin-$\frac{1}{2}$ particle to be an electron moving in the central Coulomb potential of a point nucleus of charge number Z,

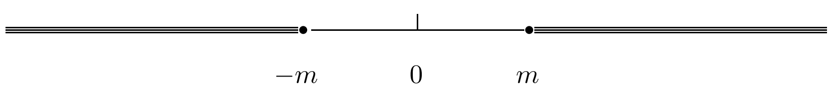
$$V \;=\; -\frac{\gamma}{x}, \qquad\qquad \gamma \;=\; Z\,e^2,$$

where $x := |\mathbf{x}|$ and in our units, $e^2 \approx 1/137.04$ is the fine-structure constant. The required $|D_0|$-form boundedness of V leads to a restriction of the potential strength γ.

The spectrum of an operator H gives information about the energy values which the particle can have when it moves in the potential V. It is the set

$$\sigma(H) := \;\{\lambda \in \mathbb{R} :\; H \,-\, \lambda\,\mathrm{id} \quad \text{is not boundedly invertible}\},$$

i.e., $\sigma(H)$ is the complement of the subset $\lambda \in \mathbb{R}$ for which $H - \lambda\,\mathrm{id}$ is bijective with a bounded inverse (id is the identity operator). For a free particle ($V = 0$), the spectrum of the Dirac operator consists of two half-lines, $(-\infty, m] \,\cup\, [m, \infty)$



separated by a gap of $2m$ (in our units, m is the rest energy of the particle; states above m are electronic states, while states below $-m$ are allocated to positrons). From this it follows that the Dirac operator is unbounded both from above and from below. When the potential is switched on, bound eigenstates appear with energies E_i lying in the gap. The eigenvalue equation $H\varphi_i = E_i\varphi_i$ is exactly solvable for the point-nucleus Coulomb potential, with its lowest (ground-state) energy given by (Darwin 1928, see also Rose 1961)

$$E_0 \;=\; m\,\sqrt{1 - Z^2e^4}\,,$$

yielding $E_0 \geq 0$ for $\gamma = Ze^2 \leq 1$. This exact reference value can be used to test our perturbative approach given below. Beyond that our method can be applied to Coulomb-type potentials where no exact solutions exist (such as sums of Coulombic and short-range potentials occurring in the single-particle models for multi-electron ions).

In electron spectroscopy the energies involved are usually much smaller than the gap such that the creation of electron-positron pairs, described in terms of excitation of a state with energy smaller than $-m$ to a state lying above m (or to an unoccupied bound state with positive energy), is negligible.

As long as only electrons (but not positrons) are considered, it is of disadvantage to describe them in terms of an operator which is unbounded from below. For the determination of the energy eigenstates the common simple variational principles, based on minimising the energy expectation value, cannot be used any more. Instead, so-called minimax procedures are required (Dolbeault, Esteban and Séré 2000 and references therein), or different methods have to be found.

Historically, several tools were employed to get rid of the negative-energy continuum and to derive from the Dirac operator a pseudo-relativistic operator which is bounded from below. Pauli, based on his two-component pre-Dirac theory which incorporates relativistic effects (Pauli 1927), introduced a systematic procedure for the elimination of the two small (positron-like) components of the 4-spinor obeying the Dirac eigenvalue equation (see, e.g., Pauli 1958). The resulting equation for a function composed of the remaining two (large, i.e., electron-like) components of φ is of (nonrelativistic) Schrödinger type. However, the operator defined by this Schrödinger-type equation has some serious drawbacks, e.g., the operators in certain orders of Ze^2 are no longer symmetric. The idea of reducing the Dirac operator by means of elimination and substitution methods to a semibounded operator (acting on 2-spinors) with the same ground-state properties was pursued further, see for example Durant and Malrieu (1987), DES (2000).

Another approach consisted in minimising the square of the Dirac operator (Baylis and Peel 1983), a method which works well if the potential is nonpositive.

Concerning the free ($V = 0$) Dirac operator, a major step forward was taken by Foldy and Wouthuysen (1950). They decoupled the positive and negative spectral subspaces by means of a certain unitary transformation and so obtained a semibounded, 2×2 matrix-valued operator in the electronic subspace. Also other people got involved in this project. De Vries (1970) gives an overview over related transformations and the properties of the transformed operators.

In the presence of an external field the Foldy-Wouthuysen transformation leads no longer to a complete decoupling of the two spectral subspaces. So Brown and Ravenhall (1951) suggested to project the Dirac operator onto the positive spectral subspace of the free Dirac operator D_0 by means of

$$\Lambda_+ \;=\; \frac{1}{2}\left(1 + \frac{D_0}{|D_0|}\right).$$

They obtained the operator

$$H^{(1)} := \Lambda_+ \, (D_0 \, + \, V) \, \Lambda_+$$

which is bounded from below for not too strong potentials. Formally, an operator semibounded for all potentials (which admit a spectral gap) would arise from using instead of Λ_+ an exact projector P_+ which projects onto the above-gap spectral subspace of the Dirac operator with potential, $D_0 + V$. Since this projector is unknown in the case of a general potential, Douglas and Kroll (1974) introduced a perturbative approach which is based on the ideas of Foldy and Wouthuysen. It aims at decoupling the spectral subspaces of D_0 up to a given (arbitrarily chosen) order n in the potential strength γ. This is achieved by means of a series of $n+1$ consecutive unitary transformations of the Dirac operator, starting with the Foldy-Wouthuysen one. In each successive step, the transformation operator is determined by the requirement that the terms of correspondingly lowest order in γ which still couple the electron-positron subspaces are eliminated.

In the present work it is shown that the Douglas-Kroll transformation scheme is a special case of a much more general transformation scheme derived from perturbation theory (Morse and Feshbach 1953, p.1018) and developed for the study of quantum lattice systems.

The basic idea is nicely displayed in the work of Datta, Fernández and Fröhlich (1999). Assume a self-adjoint operator of the form $H = H_0 + \gamma\tilde{V}$ such that the spectrum of H_0 has bounded subsets separated by spectral gaps and let $P_i, \;\; i = 1, ..., N$ be a partition of unity, where P_i are spectral projections onto disjoint subsets of $\sigma(H_0)$. By means of a series of n unitary transformations, H is transformed into an operator which is block-diagonal up to order n in γ with respect to the spectral projections P_i. In the case of a lattice where one deals with bounded operators, it can be shown that for H_0-bounded potentials $\gamma\tilde{V}$ the perturbation series in γ converges.

In the lattice case of a discrete spectrum, the transformation operators can easily be computed. Since only (discrete) sums are involved, the defining equation for the transformation operator is algebraic with an explicit solution (see e.g. Datta, Fernández and Fröhlich 1999). If, on the other hand, the spectrum is continuous as for the Dirac operator, the corresponding sums will be singular, and a different method for solving the defining operator equation has to be used. Sobolev (2003,2004), in his study of periodic Schrödinger operators on a lattice, introduced pseudodifferential operator techniques which are readily applicable to the integral operators occurring for Coulomb-type potentials. Changing from coordinate space to momentum space where D_0 is diagonal,

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

one can represent the potentials V (as well as the transformation operators) in terms of pseudodifferential operators, defined by their symbols v, i.e.,

$$(V\,\varphi)(\mathbf{x}) := \; \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{i\mathbf{p}\mathbf{x}} \; v(\mathbf{x},\mathbf{p}) \; \hat{\varphi}(\mathbf{p}) \; d\mathbf{p}.$$

In this representation, the defining equations for the transformation operators turn into algebraic equations for their symbols, which are readily solvable. In our work we will call the general transformation scheme by means of unitary pseudodifferential operators the 'Sobolev transformation scheme'.

Wolf, Reiher and Hess (2002, 2004) have evaluated the transformed Dirac operator up to fifth order in γ for its use in quantum chemical variational calculations.

A thorough mathematical analysis has, however, only been performed for the first-order term which agrees with the Brown-Ravenhall operator defined above (Evans, Perry and Siedentop 1996, Balinksy and Evans 1998, 1999).

For the second-order pseudo-relativistic operator, introduced by Jansen and Hess (1989), only the boundedness from below for subcritical potential strength ($\gamma \leq 1.006$) is known. Also, positivity of the Jansen-Hess operator in the fictitious case of a massless particle has been shown (Brummelhuis, Siedentop and Stockmeyer 2002). The value 1.006 for the critical potential strength is very close to the exact value 1 where the ground-state energy E_0 becomes zero.

In the case of more than one particle in a central field, the intuitive way of constructing an operator which is the sum of one-particle Dirac operators $D_0^{(k)} + V^{(k)}$ plus the two-particle interaction terms, does not lead to correct results. Indeed, as was pointed out by Brown and Ravenhall (1951), one does not get stable bound-state solutions. Instead, a consistent formulation within quantum electrodynamics is required. An operator acting on 4-spinors can be derived from the full QED Hamiltonian. It can be split into a part $H_{no-pair}$ which describes stationary electronic states (conserving the number of electrons), a second part H_{pair} which accounts for pair creation, and remaining parts which additionally involve the radiation field. The mere consideration of $H_{no-pair}$ in this operator is called the 'no-pair' approximation, where one disregards pair creation and the coupling to the photon field. For the two-particle case, $N = 2$, Sucher (1958) derived the following operator (which below will be called Coulomb-Dirac operator)

$$H_{no-pair} \;=\; \sum_{k=1}^{2} (D_0^{(k)} \,+\, V^{(k)}) \;+\; P_+^{(1)}\, P_+^{(2)}\, V^{(12)}\, P_+^{(1)}\, P_+^{(2)}$$

from the Bethe-Salpeter equation of quantum electrodynamics (Bethe and Salpeter 1957). The $P_+^{(k)}$ are the exact projectors defined above, relating to the single-particle operator $D_0^{(k)} + V^{(k)}$ of particle k, and $V^{(12)}$ is the interaction between paericles 1 and 2. A nice account of the derivation of this operator is given by Douglas and Kroll (1974) who call the eigenvalue equation of $H_{no-pair}$ the Coulomb ladder equation.

Alternatively, it was later suggested (Mittleman 1981) to replace $P_+^{(k)}$ by the free projectors $\Lambda_+^{(k)}$, but to project the complete operator $\sum_{k=1}^{2} (D_0^{(k)} + V^{(k)}) + V^{(12)}$, i.e. also the single-particle contribution. This is, like the Brown-Ravenhall operator in the single-particle case, only an approximation linear in the potentials.

One aim of the present work is to get some additional information on D_0-form boundedness and the spectral properties of the (single-particle) Jansen-Hess operator for massive particles. The major goal is, however, to apply the Sobolev transformation scheme to N-electron atoms. For $N = 2$, the pseudo-relativistic operator has been derived by Douglas and Kroll (1974), and they also provide the second-order terms of the transformed electron-electron Coulomb interaction. However, within the Douglas-Kroll transformation scheme, these second-order terms are so complicated that they have been neglected in any numerical computation (Hess 1986) assuming that they are small anyway (Wolf, Reiher and Hess 2004). Application of the Sobolev transformation scheme provides a breakthrough in the respect that the resulting transformed second-order operators have a very simple structure. Thus a detailed mathematical analysis becomes feasible.

The lay-out of the present work is as follows. After an overview of some basic auxiliary theorems and of the pseudodifferential operator technique (section I.1), the single-particle Sobolev transformation scheme is described for the Coulomb potential (section I.2), and its convergence is shown not for the Coulomb field, but for the slightly less singular potential $V = -\gamma/x^{1-\epsilon}$ $(0 < \epsilon \ll 1)$. Section I.3 furnishes the equivalence to the Douglas-Kroll transformation scheme, as well as the explicit form of the transformed operator to second order in γ in either representation. Subsequently, D_0-form boundedness of the potential terms of the Jansen-Hess operator is shown as well as subordinacy of the second-order terms with respect to the first-order terms for sufficiently small potential strength. Also, positivity is proven, although we did not succeed in showing it for the same range of γ as in the massless case (section I.4). The single-particle investigations are terminated with the localisation of the essential spectrum of the Jansen-Hess operator at $[m, \infty)$, with the proof of the absence of singular continuous spectrum as well as the absence of embedded eigenvalues in $[m, \infty)$ up to certain critical coupling strengths, and finally with showing the absolute continuity of the spectrum for the fictitious massless particle. These results are a generalisation of those known for the Brown-Ravenhall operator.

Part II deals with the two-particle Coulomb-Dirac operator. In this case, the second unitary transformation contains a correlated two-particle contribution (the boundedness of which is proven in section II.3) which, however, does not enter into the transformed second-order operator (section II.4). Again, the relative form boundedness of the transformed potential terms as well as positivity of the resulting pseudo-relativistic operator is proven for subcritical potential strength. The maximum possible potential strength for these properties to hold, derived from the present type of estimates, is slightly below the one for the single-particle operator. Part II is closed by localising the essential spectrum of the pseudo-relativistic two-particle operator. With the help of its behaviour under translations it is found that the essential spectrum of the free two-particle operator, $[2m, \infty)$, is a subset of the essential spectrum of the transformed two-particle operator with all potential terms included. The essential spectrum of the latter does not change when the transformed two-particle second-order potential is dropped. The proof of the conjecture that the infimum of the essential spectrum of a two-electron ion is given by the ground-state energy of the corresponding one-electron ion, increased by the rest energy of the second electron (the relativistic version of the HVZ theorem (Reed-Simon 1978, Theorem XIII.17)) is left to future investigations.

We close our work by deriving the second-order pseudo-relativistic operator in the N-particle case, $N > 2$ (part III). To this order it turns out to be a simple generalisation of the operator derived for $N = 2$, and hence its positivity is readily shown. In the case of neutral atoms ($N = Z$) the corresponding critical potential strength is found to be considerably smaller than for one- or two-electron ions. Its reduction for $N = Z$ is a consequence of the additional presence of the second-order two-particle interaction terms which scale with N^2. Although controlled by the first-order electron-electron interaction, these terms are conjectured to be of opposite sign. Hence their neglect in quantum chemical calculations should be questioned.

I. One-Electron Ions and the Jansen-Hess Operator

Let $D_0 = \boldsymbol{\alpha}\mathbf{p} + \beta m$ be the free one-particle Dirac operator with $\mathbf{p} := -i\partial/\partial\mathbf{x}$. It is defined in the Hilbert space $L_2(\mathbb{R}^3) \times \mathbb{C}^4$, and it is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^4$ where $\mathcal{S}$ is the Schwartz space of smooth strongly decreasing functions (Werner 1995, p.167). This dense subspace will be used when certain analyticity or convergence properties of the 4-spinors are required. The domain $\mathcal{D}(D_0)$ on which D_0 is self-adjoint, is $H_1(\mathbb{R}^3) \times \mathbb{C}^4$. The Sobolev spaces of order σ can be characterised in the following manner.

Let $f : \mathbb{R}^3 \to \mathbb{R}$ be defined by $f(\mathbf{p}) := (1+p^2)^{1/2}$, and consider for $\varphi \in \mathcal{S}$ the Fourier transform

$$(\widehat{f^\sigma \varphi})(\mathbf{p}) \;=\; (1+p^2)^{\frac{\sigma}{2}}\; \hat{\varphi}(\mathbf{p}), \tag{I.1}$$

which can be continuously extended to $\mathcal{S}'$, the dual space of $\mathcal{S}$. Here, $p := |\mathbf{p}|$ is the modulus of $\mathbf{p}$ and $\hat{\varphi}$ denotes the Fourier transform of φ. Define the space $H_\sigma(\mathbb{R}^3)$ by means of

$$H_\sigma(\mathbb{R}^3) := \{\varphi \in \mathcal{S}' :\; f^\sigma\, \varphi \in L_2(\mathbb{R}^3)\} \tag{I.2}$$

with the scalar product

$$(\varphi, \psi)_\sigma := \;(f^\sigma\, \varphi, f^\sigma\, \psi) \;=\; \int_{\mathbb{R}^3} (1+p^2)^\sigma\; \overline{\hat{\varphi}(\mathbf{p})}\; \hat{\psi}(\mathbf{p})\; d\mathbf{p}. \tag{I.3}$$

These Sobolev spaces are Hilbert spaces and are dense subspaces of $L_2(\mathbb{R}^3)$. In turn, $\mathcal{S}$ is dense in $H_\sigma(\mathbb{R}^3)$ (Werner 1995, §V.2; Folland 1995, p.192). Our cases of interest are $\sigma = 1$ and $\sigma = 1/2$. The space $H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4$ is the form domain of D_0.

The one-electron Dirac operator is defined by $H = D_0 + V$ with $V := -\gamma/x$ where $x := |\mathbf{x}|$. For subcritical potential strengths $\gamma < \sqrt{3}/2$ one has $\mathcal{D}(H) = \mathcal{D}(D_0)$ with H being self-adjoint on $\mathcal{D}(D_0)$ and for $\gamma < 1$, H has a self-adjoint extension (Thaller 1992, p.114).

I.1. **Preliminaries.**

This section contains a compilation of some auxiliary theorems which will be frequently used in the following. They concern estimates of essentially self-adjoint operators from above, in the form as well as in the norm sense. They are formulated for single-particle operators, but they are readily generalised to the multi-particle case (see part II). Also, the pseudodifferential operator calculus will be introduced.

a) Auxiliary theorems

In all subsequent formulae, integration over three-dimensional coordinates or momenta extends over the whole space $\mathbb{R}^3$.

Lemma I.1 (Lieb and Yau formula).
Let $k(\mathbf{p},\mathbf{p}') = k(\mathbf{p}',\mathbf{p}) \geq 0$ be a symmetric kernel, $\mathbf{p},\mathbf{p}' \in \mathbb{R}^3$. Let $f(p) > 0$ for $p > 0$ be a smooth convergence generating function. Then for $\varphi \in \mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^n$ with $n \in \mathbb{N}_0$ and $\mathcal{S}$ the Schwartz space, one has

$$\left| \int d\mathbf{p}\; d\mathbf{p}'\; \overline{\varphi(\mathbf{p})}\; k(\mathbf{p},\mathbf{p}')\; \varphi(\mathbf{p}') \right| \;\leq\; \int d\mathbf{p}\; |\varphi(\mathbf{p})|^2\; I(p)$$

$$I(p) := \;\int d\mathbf{p}'\; k(\mathbf{p},\mathbf{p}')\; \frac{f(p)}{f(p')}. \tag{I.1.1}$$

The lemma is easily derived from the Schur test for the boundedness of integral operators (see e.g. Halmos and Sunder 1978, p.22). It can be proved with the help of the Schwarz inequality (Lieb and Yau 1988, EPS 1996).

Lemma I.2 (Lieb and Yau formula for arbitrary kernels)**.**
Let A be an integral operator defined by the kernel $k(\mathbf{p},\mathbf{p}')$,

$$(A\varphi)(\mathbf{p}) \;=\; \int d\mathbf{p}'\; k(\mathbf{p},\mathbf{p}')\;\varphi(\mathbf{p}'). \tag{I.1.2}$$

Let $f(p)>0$ for $p>0$ and $\varphi,\psi\in\mathcal{S}(\mathbb{R}^3)\times\mathbb{C}^n,\;\; n\in\mathbb{N}_0$. Then

$$|(\varphi,A\,\psi)| \;=\; \left|\int d\mathbf{p}\,d\mathbf{p}'\,\overline{\varphi(\mathbf{p})}\,k(\mathbf{p},\mathbf{p}')\,\psi(\mathbf{p}')\right|$$

$$\le\; \left(\int d\mathbf{p}\,|\varphi(\mathbf{p})|^2\,I_1(p)\cdot\int d\mathbf{p}\,|\psi(\mathbf{p})|^2\,I_2(p)\right)^{\frac12} \tag{I.1.3}$$

$$I_1(p) := \int d\mathbf{p}'\,|k(\mathbf{p},\mathbf{p}')|\,\frac{f(p)}{f(p')},\qquad I_2(p) := \int d\mathbf{p}'\,|k(\mathbf{p}',\mathbf{p})|\,\frac{f(p)}{f(p')}.$$

If A is essentially self-adjoint and $\varphi=\psi$, the inequality simplifies to

$$|(\varphi,A\,\varphi)| \;\le\; \int d\mathbf{p}\;|\varphi(\mathbf{p})|^2\;\tilde I_1(p) \tag{I.1.4}$$

where $\tilde I_1$ is given by I_1 with $|k(\mathbf{p},\mathbf{p}')|$ replaced by $c_0\,\tilde k(\mathbf{p},\mathbf{p}')$, an estimate of $k(\mathbf{p},\mathbf{p}')$ and its adjoint.

If $f(p)$ can be chosen in such a way that $I_1(p)$ and $I_2(p)$ are bounded for all $p\in\mathbb{R}_+$, then A is form bounded.

Proof. The l.h.s. of (I.1.3) is first estimated by $\int d\mathbf{p}d\mathbf{p}'\,|\varphi(\mathbf{p})|\,|k(\mathbf{p},\mathbf{p}')|^{\frac12}\,|k(\mathbf{p},\mathbf{p}')|^{\frac12}$ $|\psi(\mathbf{p}')|$. Introducing the factor unity $=(f(p)/f(p'))^{\frac12}(f(p')/f(p))^{\frac12}$ as in the proof of Lemma I.1, (I.1.3) results from the Schwarz inequality.

Symmetric operators fulfilling $(\varphi,A\varphi)=(A\varphi,\varphi)$ can readily be shown from (I.1.2) to have kernels with $k(\mathbf{p},\mathbf{p}')=k^*(\mathbf{p}',\mathbf{p})$. Both $|k(\mathbf{p},\mathbf{p}')|$ and $|k^*(\mathbf{p},\mathbf{p}')|$ can be estimated by $c_0\tilde k(\mathbf{p},\mathbf{p}')$ where $\tilde k(\mathbf{p},\mathbf{p}')$ is a nonnegative function characterising the symbol class of A (to be explained in subsection b). Hence, both $I_1(p)$ and $I_2(p)$ can be estimated by the same integral, which proves (I.1.4). ■

Lemma I.3 (Operator boundedness for form bounded operators)**.**
Let A be an essentially self-adjoint operator acting on $\mathcal{S}(\mathbb{R}^3)\times\mathbb{C}^n,\;\; n\in\mathbb{N}_0$. Suppose that A is form bounded with form bound c where c is obtained with the help of Lemma I.2. Then

$$\|A\,\varphi\|^2 \;\le\; c^2\;(\varphi,\varphi). \tag{I.1.5}$$

The condition on c can be dropped if A extends to a nonnegative operator.

Hence, under the above assumption operator boundedness is a consequence of form boundedness. Note that the reverse (with the same constant c) is always true, since one has $|(\varphi,A\varphi)|\le\|A\varphi\|\cdot\|\varphi\|\le c\,\|\varphi\|^2$, if $\|A\|\le c$ is bounded.

Proof. In the special case that A extends to a form bounded, self-adjoint operator with $A\ge 0$, the proof is very simple. With $A=A^{\frac12}\cdot A^{\frac12}$ and consequently $\|A\|\le\|A^{\frac12}\|^2$, one has

$$\|A\| \;=\; \sup_{\|\varphi\|=1}\|A\,\varphi\| \;\le\; \sup_{\|\varphi\|=1}\|A^{\frac12}\varphi\|^2 \;=\; \sup_{\|\varphi\|=1}(\varphi,A\,\varphi)\;\le\; c. \tag{I.1.6}$$

Now let A be an arbitrary symmetric operator defined by (I.1.2). Then, applying the Lieb and Yau formula (I.1.4),

$$\|A\,\varphi\|^2 \;\leq\; \int d\mathbf{p}\,d\mathbf{q}'\;|\varphi(\mathbf{q}')|\;|k^*(\mathbf{p},\mathbf{q}')|\;\int d\mathbf{p}'\;|k(\mathbf{p},\mathbf{p}')|\;|\varphi(\mathbf{p}')|$$

$$\leq\; \int d\mathbf{p}'\;|\varphi(\mathbf{p}')|^2\cdot I_N(p') \qquad \text{(I.1.7)}$$

$$I_N(p') \;:=\; c_0^2\int d\mathbf{q}'\,d\mathbf{p}\;\tilde{k}(\mathbf{p}',\mathbf{p})\cdot\tilde{k}(\mathbf{p},\mathbf{q}')\;\frac{f(p')}{f(q')}$$

with $\tilde{k}$ from Lemma I.2. By assumption, A is form bounded with form bound c, i.e.

$$|(\varphi,A\,\varphi)| \;\leq\; \int d\mathbf{p}'\;|\varphi(\mathbf{p}')|^2\;I_f(p') \qquad \text{(I.1.8)}$$

$$I_f(p') \;:=\; c_0\int d\mathbf{p}\;\tilde{k}(\mathbf{p}',\mathbf{p})\;\frac{f(p')}{f(p)}\;\leq\; c.$$

Therefore,

$$I_N(p') \;=\; c_0\int d\mathbf{p}\,\tilde{k}(\mathbf{p}',\mathbf{p})\,\frac{f(p')}{f(p)}\cdot I_f(p)\;\leq\; c_0 c\int d\mathbf{p}\,\tilde{k}(\mathbf{p}',\mathbf{p})\,\frac{f(p')}{f(p)}\;\leq\; c^2 \qquad \text{(I.1.9)}$$

such that from (I.1.7), $\|A\varphi\|^2\;\leq c^2\,\|\varphi\|^2$ which proves the lemma. ∎

Lemma I.4 (Commutativity in norm)**.**
Let A,B be essentially self-adjoint operators acting on $\mathcal{S}(\mathbb{R}^3)\times\mathbb{C}^n$, $n\in\mathbb{N}_0$ and let B be bounded. If AB is bounded with $\|AB\|\leq c$, then BA is also bounded with bound c.

Proof. We have

$$0\;\leq\;\|BA\,\varphi\|^2\;=\;(BA\,\varphi,BA\,\varphi)\;=\;(\varphi,AB\,BA\,\varphi)\;\leq\;\|\varphi\|\cdot\|AB\|\;\|BA\,\varphi\|. \qquad \text{(I.1.10)}$$

If $\|BA\,\varphi\|\;=0$ then one has trivially $\|BA\,\varphi\|\;\leq c\,\|\varphi\|$. For $\|BA\,\varphi\|\neq 0$ we get from (I.1.10)

$$\|BA\,\varphi\|\;\leq\;\|\varphi\|\cdot\|AB\|\;\leq\;c\,\|\varphi\|. \qquad \text{(I.1.11)}$$

∎

The proof is the same if A is bounded instead of B.

b) Pseudodifferential operators

Pseudodifferential operators (ΨDO's) are defined in terms of a generalised Fourier transformation of a function φ. Let for the present case of interest $\varphi\in\mathcal{S}(\mathbb{R}^3)\times\mathbb{C}^4$. A pseudodifferential operator A is defined through its symbol $a(\mathbf{x},\mathbf{p}):\mathbb{R}^3\times\mathbb{R}^3\to\mathbb{C}^{4,4}$, a complex matrix-valued function, by means of (Taylor 1981)

$$(A\varphi)(\mathbf{x}) := \frac{1}{(2\pi)^{3/2}}\int d\mathbf{p}\;e^{i\mathbf{p}\mathbf{x}}\;a(\mathbf{x},\mathbf{p})\;\hat{\varphi}(\mathbf{p}). \qquad \text{(I.1.12)}$$

Since the free Dirac operator $D_0\;=\;\boldsymbol{\alpha}\mathbf{p}+\beta m$ is a multiplication operator in momentum space, it is convenient to set up the ΨDO calculus in Fourier space. Introducing the Fourier transform $\hat{a}(\mathbf{q},\mathbf{p})$ of the symbol $a(\mathbf{x},\mathbf{p})$, we get

$$(A\varphi)(\mathbf{x})\;=\;\frac{1}{(2\pi)^3}\int d\mathbf{p}\;e^{i\mathbf{p}\mathbf{x}}\int d\mathbf{q}\;e^{i\mathbf{q}\mathbf{x}}\;\hat{a}(\mathbf{q},\mathbf{p})\;\hat{\varphi}(\mathbf{p}). \qquad \text{(I.1.13)}$$

From this, the Fourier transform of $A\varphi$ is found to be

$$(\widehat{A\varphi})(\mathbf{p})\;=\;\frac{1}{(2\pi)^{3/2}}\int d\mathbf{p}'\;\hat{a}(\mathbf{p}-\mathbf{p}',\mathbf{p}')\;\hat{\varphi}(\mathbf{p}'). \qquad \text{(I.1.14)}$$

If A can be extended to a self-adjoint operator satisfying $(\varphi, A\varphi) = (A\varphi, \varphi)$, its symbol and its adjoint are related by means of

$$\hat{a}(-\mathbf{q}, \mathbf{p}+\mathbf{q})^* = \hat{a}(\mathbf{q}, \mathbf{p}). \tag{I.1.15}$$

For later use we define the symbol of a product of operators A, B. Replacing formally φ in (I.1.13) by $B\varphi$, one obtains

$$(A\,B\,\varphi)(\mathbf{x}) = \frac{1}{(2\pi)^3} \int d\mathbf{p}\; e^{i\mathbf{px}} \int d\mathbf{p}'\; \hat{a}(\mathbf{p}-\mathbf{p}', \mathbf{p}')\; \widehat{B\varphi}(\mathbf{p}'). \tag{I.1.16}$$

Inserting (I.1.14) for $\widehat{B\varphi}(\mathbf{p})$, one gets for the Fourier transformed symbol $\widehat{ab}$ of AB,

$$\widehat{ab}(\mathbf{q}, \mathbf{p}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p}'\; \hat{a}(\mathbf{q}-\mathbf{p}', \mathbf{p}+\mathbf{p}')\; \hat{b}(\mathbf{p}', \mathbf{p}). \tag{I.1.17}$$

The estimate of a symbol defines its so-called symbol class (Taylor 1981, Sobolev 2004). To estimate the symbol a (in momentum space) means that we classify $\hat{a}(\mathbf{q}, \mathbf{p})$ by its asymptotic behaviour for $q, p \to 0$ and $q, p \to \infty$ where q and p are the moduli of $\mathbf{q}$ and $\mathbf{p}$, respectively. A necessary condition is that $\hat{a}$ is a continuous function of q and p in $\mathbb{R}_+ \times \mathbb{R}_+$.

We note that the symbol class of a is sufficient to characterise the convergence properties of the respective integrals involving the symbol of A.

I.2. **The Sobolev transformation scheme.**

Our aim is to transform the one-particle Dirac operator by means of a series of unitary transformations such that the resulting operator does not couple the positive and negative spectral subspaces of the free Dirac operator D_0. Unitary transformations do not change the expectation value and hence the spectrum of the operator; however, different unitary transformations may lead to different operators. The decoupling of the spectral subspaces can be achieved up to any given order in the potential strength γ. First we define the transformations, then we show that the well-known Brown-Ravenhall operator, linear in γ, is reproduced. Subsequently we set up the transformed Dirac operator and prove boundedness of the operators which define the unitary transformations. Finally we show the subdominance of the higher-order potential terms in the case of the potential $V = -\gamma/x^{1-\epsilon}$, which is slightly less singular than the Coulomb field.

Our basic result is formulated in the following theorem.

Theorem I.1.
Let $H = D_0 + V$ be the one-particle Dirac operator acting on $\mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^4$ with $\mathcal{S}$ the Schwartz space of smooth strongly localised functions. Let γ be the strength of the potential V. 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

$$(U_1 \cdots U_n)^{-1}\, H\, U_1 \cdots U_n = H^{(n)} + R(\gamma^{n+1}) \tag{I.2.1}$$

$$H^{(n)} = \Lambda_+ \left(\sum_{k=0}^{n} H_k \right) \Lambda_+ + \Lambda_- \left(\sum_{k=0}^{n} H_k \right) \Lambda_-. \tag{I.2.2}$$

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 $R(\gamma^{n+1})$ which still couples the spectral subspaces of D_0 is p-form bounded with form bound proportional to γ^{n+1}. The operators B_k are symmetric and bounded, extending to self-adjoint operators on $L_2(\mathbb{R}^3) \times \mathbb{C}^4$.

An operator H_k with the properties stated in the theorem is said to be *of order* γ^k.

a) Unitary transformations

Let $U_k(t) = e^{iB_k t}$, $t \in \mathbb{R}$ be a group of unitary operators and consider $U_k = e^{iB_k}$ as an element of this group.

Let A be an arbitrary t-independent operator. The derivative of the transformed operator is given by

$$\frac{d}{dt}A(t) := \frac{d}{dt}\left(e^{-iB_k t}\, A\, e^{iB_k t}\right) = i\, U_k(-t)\, [A, B_k]\, U_k(t) \tag{I.2.3}$$

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

$$A(t) = U_k(-t)\, A\, U_k(t) = A + i \int_0^t d\tau\; U_k(-\tau)\, [A, B_k]\, U_k(\tau). \tag{I.2.4}$$

Iterating once, i.e. replacing A in (I.2.4) by the operator $[A, B_k]$ and inserting the resulting equation into the r.h.s. of (I.2.4), one obtains for $t = 1$

$$A(1) = A + i[A, B_k] + i^2 \int_0^1 d\tau \int_0^\tau dt'\, U_k(-t')\, [[A, B_k], B_k]\, U_k(t'). \tag{I.2.5}$$

After $n-1$ iterations the following representation of $A(1) = e^{-iB_k}\, A\, e^{iB_k}$ is obtained,

$$A(1) = A + i[A, B_k] + \frac{1}{2!} i^2\, [[A, B_k], B_k] + ... + \frac{1}{n!} i^n\, [[...[A, B_k], ..., B_k] + R \tag{I.2.6}$$

where the n-th term consists of 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 I.1,

$$(U_1 \cdots U_{n-1})^{-1}\, H\, U_1 \cdots U_{n-1} = H^{(n-1)} + H_n + R(\gamma^{n+1}) \tag{I.2.7}$$

where H_n is of order γ^n and still couples the spectral subspaces. R is a generic notation for the remainder. Decompose H_n into

$$H_n = V_n + W_n, \qquad V_n := \Lambda_+ H_n \Lambda_+ + \Lambda_- H_n \Lambda_-$$
$$W_n := \Lambda_+ H_n \Lambda_- + \Lambda_- H_n \Lambda_+\,. \tag{I.2.8}$$

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 (I.2.6), 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

$$U_n^{-1}\, (H^{(n-1)} + H_n)\, U_n = H^{(n-1)} + V_n + W_n + i[D_0, B_n] \tag{I.2.9}$$
$$+\, i\, [(\Lambda_+ \sum_{k=1}^{n-1} H_k \Lambda_+ + \Lambda_- \sum_{k=1}^{n-1} H_k \Lambda_-),\, B_n] + R(B_n^2).$$

B_n is determined from the requirement

$$W_n + i\,[D_0, B_n] = 0. \tag{I.2.10}$$

Since W_n is of order γ^n, B_n is proportional to γ^n. 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 R is of order γ^{2n}. Hence, these terms are disregarded (together with the remainder $R(\gamma^{n+1})$ from (I.2.7)) in constructing the transformed operator to order n,

$$H^{(n)} \;=\; H^{(n-1)} \,+\, V_n \;=\; D_0 \,+\, V_1 \,+\, V_2 \,+\, ... + V_n. \tag{I.2.11}$$

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

$$H^{(1)} \;=\; D_0 \,+\, V_1 \;=\; \Lambda_+ \, (D_0 + V) \, \Lambda_+ \,+\, \Lambda_- \, (D_0 + V) \, \Lambda_-. \tag{I.2.12}$$

Restricting $H^{(1)}$ to the positive spectral subspace $\mathcal{H}_{+,1}$, the second term on the r.h.s. of (I.2.12) vanishes and the remaining term agrees with the Brown-Ravenhall operator analysed by EPS (1996).

Let us now consider $n = 2$. From (I.2.11) 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

$$U_1^{-1} \, H \, U_1 \;=\; D_0 + V_1 + W_1 \,+\, i\,[D_0, B_1] \,+\, i\,[V, B_1] \,-\, \frac{1}{2}[[D_0, B_1], B_1] \,+\, R(\gamma^3),$$

$$R(\gamma^3) \;=\; -\int_0^1 d\tau \int_0^\tau dt' \; U_1(-t') \; [[V, B_1], B_1] \; U_1(t') \tag{I.2.13}$$

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

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

$$H^{(2)} \;=\; D_0 + V_1 \,+\, \Lambda_+ H_2 \Lambda_+ \,+\, \Lambda_- H_2 \Lambda_- \tag{I.2.14}$$

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

When restricted to $\mathcal{H}_{+,1}$, the first contribution to H_2 vanishes (see section I.3).

b) Determination of B_1 and its existence

We will consider the operators B_n, $n = 1, 2...$ as pseudodifferential operators, defined by means of their symbols, ϕ_n. These symbols will be derived in momentum space from a solution of (I.2.10). The result for B_1 is described in the following lemma.

Lemma I.5 (Characterisation of the transformation $U_1 = e^{iB_1}$).
The symbol ϕ_1 of B_1 is given by

$$\hat{\phi}_1(\mathbf{q}, \mathbf{p}) \;=\; -\frac{i\gamma_0}{q^2} \, \frac{1}{E_p + E_{|\mathbf{q}+\mathbf{p}|}} \, (\tilde{D}_0(\mathbf{q} + \mathbf{p}) \,-\, \tilde{D}_0(\mathbf{p})) \tag{I.2.15}$$

with $\gamma_0 := \gamma/\sqrt{2\pi}$ and

$$\tilde{D_0}(\mathbf{p}) := \frac{D_0(\mathbf{p})}{|D_0(\mathbf{p})|}, \qquad |D_0(\mathbf{p})| \;=\; E_p \;=\; \sqrt{p^2 + m^2}\,. \tag{I.2.16}$$

Its symbol class is determined by

$$|\hat{\phi}_1(\mathbf{q}, \mathbf{p})| \;\leq\; \frac{c}{q} \, \frac{1}{(q + p + 1)^2} \tag{I.2.17}$$

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

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

One has to solve

$$-i\,[D_0, B_1] \;=\; W_1 \;=\; \frac{1}{2}\,(V \;-\; \tilde{D}_0\,V\,\tilde{D}_0). \tag{I.2.18}$$

We consider the operators B_1, V, D_0 as ΨDO's according to (I.1.13). From the Fourier transforms of D_0 and V one gets for $\varphi \in \mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^4$,

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

$$(V\,\varphi)(\mathbf{x}) \;=\; \frac{1}{(2\pi)^{3/2}} \int d\mathbf{q}\; e^{i\mathbf{qx}} \left(-\frac{\gamma}{2\pi^2 q^2}\right) \int d\mathbf{p}\; e^{i\mathbf{px}}\,\hat{\varphi}(\mathbf{p}) \tag{I.2.19}$$

such that the symbol v of V is defined by $\hat{v}(\mathbf{q},\mathbf{p}) = -\sqrt{2/\pi}\,\gamma/q^2$. Moreover,

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

$$=\; \frac{1}{(2\pi)^3} \int d\mathbf{p}\,d\mathbf{q}\,[\boldsymbol{\alpha}(\mathbf{p}+\mathbf{q}) \;+\; \beta m]\;e^{i(\mathbf{p}+\mathbf{q})\mathbf{x}}\;\hat{\phi}_1(\mathbf{q},\mathbf{p})\;\hat{\varphi}(\mathbf{p}). \tag{I.2.20}$$

Acting (I.2.18) on φ and equating the respective symbols leads to the following algebraic equation for $\hat{\phi}_1$:

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

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

$\hat{w}_1(\mathbf{q},\mathbf{p})$, behaving like q^{-1} for $q \to 0$, is less singular than $\hat{v}(\mathbf{q},\mathbf{p})$, such that the prescription (I.2.8) for W_1 implies a regularisation of the potential V.

In order to solve (I.2.21) the ansatz is made

$$\hat{\phi}_1(\mathbf{q},\mathbf{p}) \;=\; -\frac{i\gamma_0}{q^2}\,(c_1\boldsymbol{\alpha}\mathbf{q} \;+\; c_2\boldsymbol{\alpha}\mathbf{p} \;+\; c_3\beta) \tag{I.2.22}$$

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

$$\boldsymbol{\alpha}\mathbf{p}\cdot\boldsymbol{\alpha}\mathbf{p} \;=\; p^2, \qquad\qquad \boldsymbol{\alpha}\mathbf{q}\cdot\boldsymbol{\alpha}\mathbf{p} \;=\; 2\mathbf{pq} \;-\; \boldsymbol{\alpha}\mathbf{p}\cdot\boldsymbol{\alpha}\mathbf{q}. \tag{I.2.23}$$

Insertion of (I.2.22) into (I.2.21) then leads to an equation of the type

$$\lambda_1\,\boldsymbol{\alpha}\mathbf{p}\cdot\boldsymbol{\alpha}\mathbf{q} \;+\; \lambda_2\,\boldsymbol{\alpha}\mathbf{q}\cdot\beta \;+\; \lambda_3\,\boldsymbol{\alpha}\mathbf{p}\cdot\beta \;+\; \lambda_4 \;=\; 0 \tag{I.2.24}$$

where the $\lambda_k,\ \ k = 1,...,4,$ are scalars depending on $\mathbf{p}$ and $\mathbf{q}$. (I.2.24) 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,

$$c_1\,(q^2 + 2\mathbf{pq}) \;=\; 1 - \frac{E_p}{E_{|\mathbf{q}+\mathbf{p}|}}, \qquad c_2 \;=\; 2c_1 - \frac{1}{E_p\,E_{|\mathbf{q}+\mathbf{p}|}}, \qquad c_3 \;=\; c_2 m \tag{I.2.25}$$

such that

$$\hat{\phi}_1(\mathbf{q},\mathbf{p}) = -\frac{i\gamma_0}{q^2}\left\{[(\mathbf{q}+2\mathbf{p})\boldsymbol{\alpha} \;+ 2\beta m]\,\frac{1}{q^2 + 2\mathbf{pq}}\left(1 \;-\; \frac{E_p}{E_{|\mathbf{q}+\mathbf{p}|}}\right) \;-\; \frac{\mathbf{p}\boldsymbol{\alpha} + \beta m}{E_p\,E_{|\mathbf{q}+\mathbf{p}|}}\right\}. \tag{I.2.26}$$

It is readily verified that (I.2.26) can be cast into the form

$$\hat{\phi}_1(\mathbf{q},\mathbf{p}) \;=\; -\frac{i\gamma_0}{q^2}\,\frac{1}{E_p + E_{|\mathbf{q}+\mathbf{p}|}}\left\{\frac{\boldsymbol{\alpha}\mathbf{q}}{E_{|\mathbf{q}+\mathbf{p}|}} \;+\; [\boldsymbol{\alpha}\mathbf{p} \;+\; \beta m]\left(\frac{1}{E_{|\mathbf{q}+\mathbf{p}|}} \;-\; \frac{1}{E_p}\right)\right\} \tag{I.2.27}$$

from which the claim (I.2.15) of the lemma is obvious.

(ii) Symbol class of ϕ_1

It is seen from (I.2.27) that $\hat{\phi}_1(\mathbf{q},\mathbf{p})$ is continuous in both variables except for $q=0$. Moreover, $\hat{\phi}_1(\mathbf{q},\mathbf{p})$ is finite but nonzero for $p=0$ and diverges like $1/q$ for $q\to 0$, while asymptotically, it decreases like $1/q^3$ respective $1/p^2$. Taken into consideration that B_1 is dimensionless (since $U_1=e^{iB_1}$) and so is $\phi_1(\mathbf{x},\mathbf{p})$, one finds that $\hat{\phi}_1(\mathbf{q},\mathbf{p})$ is of dimension (momentum)$^{-3}$ and hence is estimated by $|\hat{\phi}_1(\mathbf{q},\mathbf{p})| \le c/q\cdot(q+p+1)^{-2}$.

(iii) Boundedness of B_1

We present the proof of the form boundedness of B_1; the operator boundedness of B_1 follows from Lemma I.3.

The basic ingredient is the Lieb and Yau formula from Lemma I.2. From (I.2.27) one has $\hat{\phi}_1^*(\mathbf{q},\mathbf{p})=-\hat{\phi}_1(\mathbf{q},\mathbf{p})$ since $\boldsymbol{\alpha}$ and β are self-adjoint, such that (I.1.4) can be used with the constant $c_0=1$ and $\tilde{k}=k$. Starting from (I.1.14), applying (I.1.4) and subsequently inserting the symbol class (I.2.17) of ϕ_1, one obtains for $\varphi\in L_2(\mathbb{R}^3)\times\mathbb{C}^4$ the estimate

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

$$\le\; \frac{c}{(2\pi)^{\frac{3}{2}}}\int d\mathbf{p}\,|\hat{\varphi}(\mathbf{p})|^2\;\cdot I_1(p) \qquad \text{(I.2.28)}$$

$$I_1(p) := \int d\mathbf{q}\,\frac{1}{|\mathbf{q}-\mathbf{p}|}\,\frac{1}{(|\mathbf{q}-\mathbf{p}|\,+p+1)^2}\,\frac{f(p)}{f(q)}.$$

It remains to prove that $I_1(p)$ is bounded for $p\in\mathbb{R}_+$. For the convergence generating function, the choice $f(p):=p$ is made. Performing the angular integration with the help of Appendix A, one obtains

$$I_1(p) \;=\; 2\pi\int_0^\infty dq\,\left(\frac{1}{|q-p|\,+p+1} \;-\; \frac{1}{q+2p+1}\right) \;=\; 4\pi\,\ln\frac{2p+1}{p+1}\;<\infty\,. \qquad \text{(I.2.29)}$$

Hence B_1, and also $U_1=e^{iB_1}$, is a bounded operator on $L_2(\mathbb{R}^3)\times\mathbb{C}^4$.

(iv) Self-adjointness of B_1

Taking the adjoint of the defining equation (I.2.18) and using that D_0 and W_1 extend to self-adjoint operators, leads to $W_1=-i[D_0,B_1^*]$, which agrees with (I.2.18) for $B_1^*=B_1$. In fact, from the explicit form (I.2.27) of $\hat{\phi}_1$, the symmetry condition (I.1.15) follows immediately. Self-adjointness of B_1 is then a consequence of its boundedness. ■

c) Existence of the transformations of higher order

In order to identify the structure of the operators B_n, we set up the defining equation for $n=2$. From the definition (I.2.8) of the potential W_2, using H_2 from (I.2.14), one obtains

$$-i[D_0,B_2] = W_2 = i\Lambda_+(\,[V_1,B_1]+\frac{1}{2}[W_1,B_1]\,)\Lambda_- + i\Lambda_-(\,[V_1,B_1]+\frac{1}{2}[W_1,B_1]\,)\Lambda_+$$

$$=\;\frac{i}{8}\,\Big(3\,[V,B_1]\;+\;[\tilde{D}_0,V\tilde{D}_0\,B_1]\;+\;[\tilde{D}_0,B_1\tilde{D}_0V]\;+\;3\,\tilde{D}_0\,[B_1,V]\,\tilde{D}_0\Big) \qquad \text{(I.2.30)}$$

where $V_1=V-W_1$ was used. Thus, apart from the bounded multiplication factors $\tilde{D}_0$ (in momentum space), W_2 is determined from the commutator $[V,B_1]$. For

$n=3$, the commutators $[[V,B_1],B_1]$ and $[V,B_2]$ enter into W_3. In general, W_n is composed of multiple commutators of V with $B_k,\ \ k<n$.

In order to show the boundedness of B_n (which implies the existence of $U_n = e^{iB_n}$ as well as of $H^{(n)}$ containing commutators with $B_k,\ \ k<n$), we have to establish the p-form boundedness of the potentials W_n. Explicitly, we have to prove the following proposition.

Proposition I.1 (Existence of Sobolev transformations).
Let $U_n = e^{iB_n},\ \ n \geq 1,$ be the unitary transformations from Theorem I.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 $H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4$ by means of

$$|(\varphi, W_n\varphi)| \;\leq\; c\,(\varphi, p\,\varphi) \tag{I.2.31}$$

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

Proof.
(i) p-form boundedness of W_n
The proof is by induction. Starting with $n=1$, the p-form boundedness of W_1 from (I.2.18) follows from Kato's (1966) inequality, $(\varphi, \frac{1}{x}\varphi) \;\leq\; \frac{\pi}{2}(\varphi, p\,\varphi)$, and from the self-adjointness and boundedness of $\tilde{D}_0$ by 1,

$$|(\varphi, W_1\varphi)| \;\leq\; \frac{1}{2}\,|(\varphi, V\varphi)| \;+\; \frac{1}{2}\,|(\tilde{D}_0\varphi, V\tilde{D}_0\varphi)| \;\leq\; \frac{\gamma\pi}{4}\,(\varphi, p\,\varphi) \;+\; \frac{\gamma\pi}{4}\,(\varphi, p\,\varphi) \tag{I.2.32}$$

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

By induction hypothesis, $W_{n'}$ is p-form bounded on $H_{1/2}(\mathbb{R}^3)\times\mathbb{C}^4$ for $n' \leq n-1$. We recall that $W_{n'}$ is of the order $\gamma^{n'}$ and is composed of multiple commutators of V with $B_k,\ \ k<n'$. The orders k (in γ) of all factors $B_k,\ \ k \leq n'-1$, which enter into a given commutator contributing to $W_{n'}$ must add to $n'-1$, the last factor γ being supplied by the linearity in V. Hence, the induction hypothesis implies that all commutators of smaller order than γ^n 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 $[\cdot]$ extends to a self-adjoint operator. We symmetrise the kernel by means of $|\widehat{[\cdot]}| \;\leq\; |\widehat{[\cdot]}| + |\widehat{[\cdot]}^*|$ using that $\widehat{[\cdot]}(\mathbf{q}-\mathbf{p},\mathbf{p}) \;= \widehat{[\cdot]}^*(\mathbf{p}-\mathbf{q},\mathbf{q})$ and that symbol and its adjoint are in the same symbol class. With the help of the Lieb and Yau formula (I.1.1), the p-form boundedness of $\widehat{[\cdot]}$ can be expressed in the following way

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

$$\leq\; \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p}\ |\hat{\varphi}(\mathbf{p})|^2\ c\,p \;=\; c'\,(\varphi, p\,\varphi) \tag{I.2.33}$$

with some constant $c>0$ and $c' = c/(2\pi)^{3/2}$. The inequality in the second line of (I.2.33) restricts the convergence generating function to $f(p) := p^\lambda$ with $1<\lambda<3$. 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 $\lambda < 3$, and because $\widehat{[\cdot]}$ is of dimension $(\text{momentum})^{-2}$, decreasing like q^{-2} for $q \to \infty$, such that $\lambda > 1$ is required. These properties hold also for the symbol w_k of the self-adjoint operator W_k. Inequality (I.2.23) is therefore also valid for $\hat{w}_k$ in place of $\widehat{[\cdot]}$, if $k<n$ (when W_k is p-form bounded).

We present the proof of p-form boundedness of $[[\cdot], B_k]$; the corresponding proof for $[V, B_{n-1}]$ can be carried out along the same lines.

First we estimate the symbol ϕ_k of B_k by the symbol w_k. To do so, recall that $\hat{\phi}_k$ and $\hat{w}_k$ are interrelated by an equation of the type (I.2.21), derived from the defining equation (I.2.10) for B_k. This equation implies that the behaviour of $\hat{\phi}_k$ for $p \to 0$ and $q \to 0$ is that of $\hat{w}_k$, while there occurs an extra power of q^{-1} and p^{-1} for $q \to \infty$ and $p \to \infty$, respectively. Therefore

$$|\hat{\phi}_k(\mathbf{q}, \mathbf{p})| \;\le\; \frac{c}{q+p+1}\, |\hat{w}_k(\mathbf{q}, \mathbf{p})|. \tag{I.2.34}$$

From the essential self-adjointness of $[\cdot]$ and B_k, using the Fourier transform (I.1.14), one has

$$|(\varphi, [[\cdot], B_k]\varphi)| \;\le\; |(\widehat{[\cdot]\varphi}, \widehat{B_k\varphi})| \;+\; |(\widehat{B_k\varphi}, \widehat{[\cdot]\varphi})|$$
$$\le \frac{1}{(2\pi)^3} \int d\mathbf{p}' d\mathbf{p}\, d\mathbf{q}\; |\hat{\varphi}(\mathbf{p})| \left\{ \left| \widehat{[\cdot]}^*(\mathbf{p}' - \mathbf{p}, \mathbf{p}) \right| \; |\hat{\phi}_k(\mathbf{p}' - \mathbf{q}, \mathbf{q})| \right. \tag{I.2.35}$$
$$\left. + \; |\hat{\phi}_k^*(\mathbf{p}' - \mathbf{p}, \mathbf{p})| \; \left| \widehat{[\cdot]}(\mathbf{p}' - \mathbf{q}, \mathbf{q}) \right| \right\} |\hat{\varphi}(\mathbf{q})|.$$

According to (I.1.4)ff, the kernel of this integral can be estimated by one which is symmetric in $\mathbf{p}$ and $\mathbf{q}$, such that the Lieb and Yau formula is applicable, with the choice $f(p) = p^2$. Using subsequently the estimate (I.2.34) for ϕ_k and its adjoint, one gets

$$|(\varphi, [\,[\cdot], B_k]\,\varphi)| \;\le\; \frac{c_0}{(2\pi)^3} \int d\mathbf{p}\; |\hat{\varphi}(\mathbf{p})|^2 \;\cdot \left\{ \int d\mathbf{p}' \; \left| \widehat{[\cdot]}(\mathbf{p} - \mathbf{p}', \mathbf{p}') \right| \; \frac{p^2}{p'^2} \right.$$
$$\cdot \int d\mathbf{q}\; \frac{1}{|\mathbf{p}' - \mathbf{q}| + q + 1} \; |\hat{w}_k(\mathbf{p}' - \mathbf{q}, \mathbf{q})| \; \frac{p'^2}{q^2} \tag{I.2.36}$$
$$\left. + \int d\mathbf{p}' \; \frac{1}{|\mathbf{p} - \mathbf{p}'| + p' + 1} \; |\hat{w}_k(\mathbf{p} - \mathbf{p}', \mathbf{p}')| \; \frac{p^2}{p'^2} \int d\mathbf{q} \; \left| \widehat{[\cdot]}(\mathbf{p}' - \mathbf{q}, \mathbf{q}) \right| \; \frac{p'^2}{q^2} \right\}.$$

By virtue of (I.2.33), the second integral over $\widehat{[\cdot]}$ can be estimated by cp', respectively. Since $\hat{w}_k$ is p-form bounded, (I.2.33) can be used for $\hat{w}_k$. Thus the second term in the curly brackets can be estimated by

$$\int d\mathbf{p}' \; \frac{1}{|\mathbf{p} - \mathbf{p}'| + p' + 1} \; |\hat{w}_k(\mathbf{p} - \mathbf{p}', \mathbf{p}')| \; \frac{p^2}{p'^2} \cdot c\,p' \;\le c \int d\mathbf{p}' \; |\hat{w}_k(\mathbf{p} - \mathbf{p}', \mathbf{p}')| \; \frac{p^2}{p'^2} \;\le c' p. \tag{I.2.37}$$

In the first integral, the factor $(|\mathbf{p}' - \mathbf{q}| + q + 1)^{-1}$ is bounded for all $q \in \mathbb{R}_+$ and hence can be estimated by its value at $q = 0$. Therefore, the first term of (I.2.36) in curly brackets is estimated by

$$\int d\mathbf{p}' \; \left| \widehat{[\cdot]}(\mathbf{p} - \mathbf{p}', \mathbf{p}') \right| \; \frac{p^2}{p'^2} \cdot \frac{\tilde{c}}{p' + 1} \cdot c\,p' \;\le\; c''\, p. \tag{I.2.38}$$

Insertion into (I.2.36) proves the p-form boundedness of the commutator $[[\cdot], B_k]$.

(ii) Boundedness of B_n

This is a consequence of the p-form boundedness of W_n. From the first line of (I.2.33), with $\widehat{[\cdot]}$ replaced by $\hat{\phi}_n$, one gets with $f(p) = p^2$,

$$|(\varphi, B_n\varphi)| \;\le\; \frac{c}{(2\pi)^{3/2}} \int d\mathbf{p}\; |\hat{\varphi}(\mathbf{p})|^2 \int d\mathbf{q}\; |\hat{\phi}_n(\mathbf{p} - \mathbf{q}, \mathbf{q})| \; \frac{p^2}{q^2} \;\le\; \tilde{c}\,(\varphi, \varphi) \tag{I.2.39}$$

since according to (I.2.34) and (I.2.37), the $\mathbf{q}$-integral is bounded. ∎

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 classes, a powerful method in the case of periodic potentials (Sobolev 2003,2004).

d) p-form boundedness of the remainder $R(\gamma^{n+1})$

From its definition as remainder after multiple iterations of (I.2.5)-type equations (see e.g. (I.2.13)), $R^{(n+1)}$ 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 (I.2.10)). These commutators are p-form bounded according to the proof of Proposition I.1, and it remains to show that the unitary transform preserves the p-form boundedness. Consider

$$\begin{aligned} |(\varphi,\, U_k(-\tau)\,[\cdot]\,U_k(\tau)\,\varphi)| \;&=\; |(U_k(\tau)\,\varphi,\,[\cdot]\,U_k(\tau)\,\varphi)| \\ \leq\; c\,(U_k(\tau)\,\varphi,\,p\,U_k(\tau)\,\varphi) \;&=\; c\,(\varphi,\,U_k(-\tau)\,p\,U_k(\tau)\,\varphi). \end{aligned} \tag{I.2.40}$$

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

$$(\varphi, e^{-iB_k\tau}\,p\,e^{iB_k\tau}\,\varphi) \;\leq\; \sum_{n,m=0}^{\infty} \frac{\tau^n}{n!}\,\frac{\tau^m}{m!}\,|(\varphi, B_k^n\,p\,B_k^m\,\varphi)|. \tag{I.2.41}$$

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 (I.2.28) 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 (I.2.39),

$$I_{B_k} := \frac{1}{(2\pi)^{3/2}} \int d\mathbf{q}\,|\hat{\phi}_k(\mathbf{p}-\mathbf{q},\mathbf{q})|\,\frac{p^2}{q^2} \;\leq\; c_k. \tag{I.2.42}$$

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

(i)

$$I_{pB_k} \;=\; \frac{1}{(2\pi)^{3/2}} \int d\mathbf{q}\,p\,|\hat{\phi}_k(\mathbf{p}-\mathbf{q},\mathbf{q})|\,\frac{p^2}{q^2} \;\leq\; p\,c_k. \tag{I.2.43}$$

(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 (I.1.17) for the symbol of a product of operators. Then with (I.2.42),

$$I_{pB_k^{m+1}} \;=\; \frac{1}{(2\pi)^{3/2}} \int d\mathbf{q}'\,|\hat{s}_{pB_k^{m+1}}(\mathbf{p}-\mathbf{q}',\mathbf{q}')|\,\frac{p^2}{q'^2} \tag{I.2.44}$$

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

(iii) Decomposing $B_kpB_k^m = B_k \cdot pB_k^m$, one has from (I.2.37)

$$\begin{aligned} I_{B_kpB_k^m} \;&\leq\; \frac{1}{(2\pi)^3} \int d\mathbf{q}\,|\hat{\phi}_k(\mathbf{p}-\mathbf{q},\mathbf{q})|\,\frac{p^2}{q^2} \cdot \int d\mathbf{q}'\,|\hat{s}_{pB_k^m}(\mathbf{q}-\mathbf{q}',\mathbf{q}')|\,\frac{q^2}{q'^2} \\ &\leq\; c_k^m\,\frac{1}{(2\pi)^{3/2}} \int d\mathbf{q}\,|\hat{\phi}_k(\mathbf{p}-\mathbf{q},\mathbf{q})|\,\frac{p^2}{q} \;\leq\; c_k^m\,c_k'\,p. \end{aligned} \tag{I.2.45}$$

(iv) We claim $I_{B_k^npB_k^m} \leq p\,c_k'^n\,c_k^m$. Then, using (I.2.45)

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

$$\leq\ c_k^{'n}\, c_k^m \cdot c_k'\, p \ =\ p\, c_k^{'n+1}\, c_k^m . \tag{I.2.46}$$

Thus we obtain from the Lieb and Yau formula applied to (I.2.41)

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

$$=\ c\, e^{c_k'\tau + c_k\tau}\, (\varphi, p\,\varphi) \tag{I.2.47}$$

with c a constant resulting from using the same estimate for symbol and its adjoint. This shows that $(\varphi, U_k(-\tau)pU_k(\tau)\varphi)$ 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.

Items a) – d) constitute the proof of Theorem I.1.

e) Subordinacy of the potential terms of higher order for a modified potential

For the Coulomb field V, the total potential of the transformed Dirac operator $H^{(n)}$ to any order γ^n is p-form bounded. In fact, since V_n differs from W_n only by bounded operators (see (I.2.8)), p-form boundedness of V_n and hence of $H^{(n)} - D_0$ according to (I.2.11) follows directly from the p-form boundedness of W_n. Thus,

$$|(\varphi, (H^{(n)} - D_0)\varphi)| = |(\varphi, (V_1 + ... + V_n)\varphi)| \leq c(\varphi, p\,\varphi) \leq c(\varphi, E_p\varphi). \tag{I.2.48}$$

The form bound c is proportional to the coupling strength γ, and from the present type of estimate only smaller than 1 if $\gamma \ll 1$ is sufficiently small. Applying more elaborate methods (see section I.4) a form bound < 1 for $\gamma < 1$ has been established in the case of $V_1 + V_2$, but no further results are known.

In this section we want to investigate a slightly less singular potential,

$$V(x) :=\ -\frac{\gamma}{x^{1-\epsilon}}, \qquad \hat{v}(\mathbf{q})\ =\ -\gamma\sqrt{\frac{2}{\pi}}\,\frac{f_\epsilon}{q^{2+\epsilon}}, \quad \epsilon > 0 \tag{I.2.49}$$

where the symbol $\hat{v}(\mathbf{q},\mathbf{p}) = \hat{v}(\mathbf{q})$ is the Fourier transform and $f_\epsilon := \cos\frac{\pi\epsilon}{2}\,\Gamma(1+\epsilon) \to 1$ for $\epsilon \to 0$. For this potential it will be shown that the series $\sum_{k=1}^{\infty} V_k$ is convergent in the sense that V_{k+1} is V_k-form bounded, and that the remainder after n transformations is V_n-form bounded, all with an arbitrarily small form bound. This means that the Sobolev transformation scheme can be viewed as a proper perturbative approach for all potentials which are less singular than the Coulomb field as long as they decay at infinity sufficiently fast (such that the Fourier transform exists). Numerical investigations for the ground-state energy of one-electron ions within the Douglas-Kroll transformation scheme (to be discussed in section I.3) up to fifth order indicate convergence even in the case of a Coulomb field (Wolf, Reiher and Hess 2002).

Our results are collected in the following proposition.

Proposition I.2 (Convergence of series for modified potential)**.**
For the modified Coulomb potential (I.2.49) 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* $\varphi \in \mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^4$. *Let* $\mu_k > 0$ *for* $k \in \mathbb{N}$ *be the infimum of the constant c in the estimate* $|(\varphi, V_k\varphi)| \leq c\,(\varphi, p^{1-k\epsilon}\varphi)$. *Then* V_{k+1} *is subordinate to* V_k *in the sense*

$$|(\varphi, V_{k+1}\,\varphi)|\ \leq\ \delta\,|(\varphi, V_k\varphi)|\ +\ C\,(\varphi, \varphi) \tag{I.2.50}$$

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

(iii) *Let* $R:=(U_1\cdots U_n)^{-1}HU_1\cdots U_n - H^{(n)}$ *be the remainder of order* $n+1$ *in the potential strength. Then* R *is subordinate to* V_n.

For the proof, an auxiliary inequality is needed.

Lemma I.6. *For* $0<(n+1)\epsilon<1$, $c_0\in\mathbb{R}_+$, $n\in\mathbb{N}$ *and every* $\varphi\in H_{1/2}(\mathbb{R}^3)\times\mathbb{C}^4$ *one has*

$$c_0\,(\varphi,p^{1-(n+1)\epsilon}\varphi)\;\le\;c\,(\varphi,p^{1-n\epsilon}\varphi)\;+\;C\,(\varphi,\varphi) \tag{I.2.51}$$

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

$$c_0\,(\varphi,p^{1-\epsilon}\varphi)\;\le\;c\,(\varphi,p\,\varphi)\;+\;C\,(\varphi,\varphi). \tag{I.2.52}$$

Proof. We use an elementary inequality from analysis,

$$a\cdot b\;\le\;\frac{a^\lambda}{\lambda}\;+\;\frac{b^\mu}{\mu}\qquad\qquad\text{for } a,b>0,\quad \frac{1}{\lambda}\;+\;\frac{1}{\mu}\;=1, \tag{I.2.53}$$

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

$$p^{1-(n+1)\epsilon}\;=\;\left(\delta\,p^{1-(n+1)\epsilon}\right)\cdot\frac{1}{\delta}\;\le\;\frac{1-(n+1)\epsilon}{1-n\epsilon}\,\delta^{\frac{1-n\epsilon}{1-(n+1)\epsilon}}\,p^{1-n\epsilon}\;+\;\frac{\epsilon}{1-n\epsilon}\left(\frac{1}{\delta}\right)^{\frac{1-n\epsilon}{\epsilon}}. \tag{I.2.54}$$

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

$$c_0\,(\varphi,p^{1-(n+1)\epsilon}\varphi)\;\le\;c_0\,\delta\,(\varphi,p^{1-n\epsilon}\varphi)\;+\;c_0\,\frac{\epsilon}{1-n\epsilon}\,\delta^{-\frac{1-n\epsilon}{\epsilon}}\,(\varphi,\varphi). \tag{I.2.55}$$

With the choice $\delta:=\min\{\frac{1}{2c_0},\frac{1}{2}\}$, (I.2.51) is verified. ∎

Before we embark on the proof of the proposition, we show for $k=1$ that $|(\varphi,V_k\varphi)|\;\le\;c\,(\varphi,p^{1-k\epsilon}\varphi)$ with some constant $c>0$, such that μ_k in (ii) is well defined.

Without restriction, we can take $\mu_k>0$. In fact, assume $\mu_k=0$. Since $0<(\varphi,p^{1-k\epsilon}\varphi)<\infty$ (for $\varphi\neq 0$), the above inequality implies $(\varphi,V_k\varphi)=0$. Then V_k does not contribute to the expectation value of the transformed Dirac operator and can be disregarded altogether.

In this section, all previously defined quantities will now pertain to the modified potential (I.2.49). In order to estimate V_1, we translate (I.2.21) to the new potential and obtain for its symbol v_1

$$\hat v_1(\mathbf{q},\mathbf{p})\;=\;\hat v(\mathbf{q})\;-\;\hat w_1(\mathbf{q},\mathbf{p})\;=\;-\frac{\gamma_0}{q^{2+\epsilon}}\,f_\epsilon\,(1+\tilde D_0(\mathbf{q}+\mathbf{p})\cdot\tilde D_0(\mathbf{p})). \tag{I.2.56}$$

The multiplier of $q^{-(2+\epsilon)}$ is a bounded operator which is estimated by a constant c_1. According to (I.2.28) we obtain with $f(p):=p^2$

$$|(\varphi,V_1\,\varphi)|\;\le\;\frac{1}{(2\pi)^{3/2}}\int d\mathbf{p}\;|\hat\varphi(\mathbf{p})|^2\int d\mathbf{q}\;|\hat v_1(\mathbf{q}-\mathbf{p},\mathbf{p})|\,\frac{p^2}{q^2}. \tag{I.2.57}$$

In the latter integral, we make the substitution $p\,\mathbf{q}':=\mathbf{q}-\mathbf{p}$ and estimate with the help of Appendix A

$$c_1\int d\mathbf{q}\;\frac{1}{|\mathbf{q}-\mathbf{p}|^{2+\epsilon}}\,\frac{p^2}{q^2}\;=\;2\pi c_1\,p^{1-\epsilon}\int_0^\infty\frac{dq'}{q'^{1+\epsilon}}\;\ln\left|\frac{q'+1}{q'-1}\right|\;\le\;c\cdot p^{1-\epsilon}. \tag{I.2.58}$$

Thus $|(\varphi,V_1\varphi)|\;\le\;c_0\,(\varphi,p^{1-\epsilon}\varphi)$ with some constant c_0. Since $\mu_1=\inf c_0>0$, we have $|(\varphi,V_1\varphi)|\;>\;\frac{\mu_1}{2}\,(\varphi,p^{1-\epsilon}\varphi)$.

Proof of Proposition, (ii):
First we take $k=1$. From (I.2.14) we have $V_2 = \sum_{s=\pm} \Lambda_s(i[V_1,B_1] + \frac{i}{2}[W_1,B_1])\Lambda_s$.
As before, we disregard in the estimate of V_2 all bounded operators involving $\tilde{D}_0$ and consider V_2 as being represented by the commutator $[V,B_1]$.

We recall that the symbol of B_1 is proportional to $\hat{w}_1(\mathbf{q},\mathbf{p})$ and accordingly is estimated by $|\hat{\phi}_1(\mathbf{q},\mathbf{p})| \le \frac{c}{q^{1+\epsilon}} \frac{1}{(q+p+1)^2}$. Also, as before, $|\hat{\phi}_1^*| = |\hat{\phi}_1|$. With the substitution $\mathbf{q}' := \mathbf{q}/p'$ in the first integral we obtain, following (I.2.35) and (I.2.36),

$$|(\varphi,[V,B_1]\varphi)| \le |(\widehat{V\varphi},\widehat{B_1\varphi})| + |(\widehat{B_1\varphi},\widehat{V,\varphi})| \le \int d\mathbf{p}\, |\hat{\varphi}(\mathbf{p})|^2 \,\{I_{11}(p) + I_{12}(p)\}$$

$$I_{11}(p) = \frac{1}{(2\pi)^3}\int d\mathbf{p}'\, d\mathbf{q}\, |\hat{v}(\mathbf{p}'-\mathbf{p})|\, |\hat{\phi}_1(\mathbf{p}'-\mathbf{q},\mathbf{q})| \cdot \frac{p^2}{q^2} \tag{I.2.59}$$

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

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

For I_{11}, the $\mathbf{q}'$-integral is estimated by dropping $\frac{1}{p'}$ in the last factor of the denominator. With the substitution $\mathbf{k} := \mathbf{q}' - \hat{\mathbf{p}}'$ and Appendix A, one finds

$$\int \frac{d\mathbf{q}'}{q'^2} \frac{1}{|\mathbf{q}'-\hat{\mathbf{p}}'|^{1+\epsilon}} \frac{1}{(|\mathbf{q}'-\hat{\mathbf{p}}'| + 1)^2} = \int_0^\infty dk\, \frac{k^{1-\epsilon}}{(k+1)^2} \cdot \frac{2\pi}{k} \ln\left|\frac{k+1}{k-1}\right| < \infty. \tag{I.2.60}$$

The $\mathbf{p}'$-integral, after making the substitution $p\,\mathbf{p}'' := \mathbf{p}'$ and applying similar techniques as in (A.2), is given by

$$p^2 \int d\mathbf{p}' \frac{1}{|\mathbf{p}'-\mathbf{p}|^{2+\epsilon}} \frac{1}{p'^{2+\epsilon}} = p^{1-2\epsilon} \int_0^\infty dp'' \frac{1}{p''^{\epsilon}} \frac{2\pi}{\epsilon p''} \left(\frac{1}{|p''-1|^{\epsilon}} - \frac{1}{|p''+1|^{\epsilon}}\right)$$
$$\le c\cdot p^{1-2\epsilon}. \tag{I.2.61}$$

The second contribution, I_{12}, is estimated in a similar way and leads to the same result. Thus

$$I_{11}(p) + I_{12}(p) \le \tilde{c}\, p^{1-2\epsilon} \tag{I.2.62}$$

with some constant $\tilde{c}$. Using Lemma I.6 and the definition of μ_1, one finally obtains

$$|(\varphi,V_2\varphi)| \le c_0\,(\varphi,p^{1-2\epsilon}\varphi) \le c_0\,\delta\,(\varphi,p^{1-\epsilon}\varphi) + C\,(\varphi,\varphi) \tag{I.2.63}$$
$$< \frac{2c_0\,\delta}{\mu_1}\, |(\varphi,V_1\varphi)| + C(\varphi,\varphi)$$

with $2c_0\delta/\mu_1 < 1$ for δ chosen sufficiently small. This proves (ii) for $k=1$.

The proof of the induction step from k to $k+1$ proceeds along the same lines as applied earlier to show the p-form boundedness of W_n or V_n. By induction hypothesis commutators of order $m \le k$ in the potential strength, denoted by $[\cdot]_m$, have the following symbol estimates (compare (I.2.33))

$$\int d\mathbf{q}\, \left(\left|\widehat{[\cdot]}_m(\mathbf{q}-\mathbf{p},\mathbf{p})\right| + \left|\widehat{[\cdot]}_m^*(\mathbf{q}-\mathbf{p},\mathbf{p})\right|\right) \left(\frac{p}{q}\right)^{\lambda} \le c\, p^{1-m\epsilon} \tag{I.2.64}$$

where λ can be chosen in the interval $(1,3)$. 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 (I.2.34)

$$|\hat{\phi}_m(\mathbf{q},\mathbf{p})| \le \frac{c}{q+p+1} \left|\widehat{[\cdot]}_m(\mathbf{q},\mathbf{p})\right| \le \frac{c}{q+1} \left|\widehat{[\cdot]}_m(\mathbf{q},\mathbf{p})\right|. \tag{I.2.65}$$

Then from (I.2.35) and (I.2.36) one has with some $c_0 \in \mathbb{R}_+$,

$$|(\varphi, [[\cdot]_m, B_{k-m+1}]\,\varphi)| \;\leq\; \frac{c_0}{(2\pi)^3} \int d\mathbf{p}\; |\hat{\varphi}(\mathbf{p})|^2 \;(I_{00} \;+\; I_{01}) \tag{I.2.66}$$

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

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

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 (I.2.65). In I_{01}, the $\mathbf{q}$-integral is by (I.2.64) estimated by $c\,p'^{1-m\epsilon}$. Further one has with $a \geq 0$ and $\delta > 0$

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

$$\leq\; c\, p^{1-n\epsilon-\delta} \tag{I.2.67}$$

if $2+\delta \,< 3$. 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 (I.2.64) to estimate the $\mathbf{q}$-integral by $c\,p'^{-(k-m+1)\epsilon}$. With $\lambda := \,2+(k-m+1)\,\epsilon$ (for $(k-m+1)\epsilon \,< 1)$ in (I.2.64) 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

$$|(\varphi, [[\cdot]_m, B_{k-m+1}]\,\varphi)| \;\leq\; c_0\; (\varphi, p^{1-(k+1)\epsilon}\varphi) \tag{I.2.68}$$

which proves (I.2.64) for $k+1$. The same estimate can be shown for $|(\varphi, [V, B_k]\,\varphi)|$. Hence

$$|(\varphi, V_{k+1}\varphi)| \;\leq\; c'\; (\varphi, p^{1-(k+1)\epsilon}\varphi) \;\leq c'\,\delta\, \frac{2}{\mu_k}\; |(\varphi, V_k\varphi)| \;+\; C\;(\varphi,\varphi) \tag{I.2.69}$$

which completes the proof of (ii). ■

Proof of Proposition, (i):
We use again induction. For $k=1$, applying Lemma I.6 to the estimate of V_1,

$$|(\varphi, V_1\,\varphi)| \;\leq\; c_0\; (\varphi, p^{1-\epsilon}\,\varphi) \;\leq\; c\,(\varphi, p\,\varphi) \;+\; C\;(\varphi,\varphi) \tag{I.2.70}$$

with $c < 1$. For $k > 1$, we assume that V_k is p-form bounded with form bound $c_1 < 1$. Then we have from (ii)

$$|(\varphi, V_{k+1}\,\varphi)| \;\leq\; \delta\, |(\varphi, V_k\varphi)| \;+\; C\,(\varphi,\varphi) \;\leq\; \delta\;(c_1\,(\varphi, p\,\varphi) \;+\; C_1\,(\varphi,\varphi)) \;+\; C\,(\varphi,\varphi). \tag{I.2.71}$$

Since δ can be chosen arbitrarily small, one has $\delta c_1 < 1$. ■

A consequence of (I.2.71) is the p-form boundedness (with form bound < 1) of every finite sum $V_1 + ... + V_n$.

Proof of Proposition, (iii):
We have to show that all B_k are bounded operators. Then we can proceed as in section 2d 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 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 (I.2.50)

$$|(\varphi, R\,\varphi)| \;=\; \text{const} \cdot |(\varphi, V_{n+1}\varphi)| \;\leq\; \text{const} \cdot \delta\; |(\varphi, V_n\varphi)| \;+\; C'\;(\varphi,\varphi) \tag{I.2.72}$$

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 (I.2.42) with the substitution $\mathbf{q}' := \mathbf{q}-\mathbf{p}$,

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

$$\le \frac{c}{(2\pi)^{3/2}} \int d\mathbf{q}' \, \frac{1}{q'^{1+\epsilon}} \, \frac{1}{(q'+1)^2} \cdot \frac{p^{1-\epsilon}}{|\mathbf{p}+\mathbf{q}'|^{1-\epsilon}} \le c' \tag{I.2.73}$$

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 (I.2.45)-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 (I.2.34) 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 (I.1.17),

$$|\widehat{v\phi}_1(\mathbf{q},\mathbf{p})| \le \frac{c}{(2\pi)^{3/2}} \int d\mathbf{p}' \, \frac{1}{|\mathbf{q}-\mathbf{p}'|^{2+\epsilon}} \cdot \frac{1}{p'^{1+\epsilon}(p'+p+1)^2}. \tag{I.2.74}$$

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 Appendix A such that one gets for $q \neq 0$, $\epsilon \neq 0$,

$$|\widehat{v\phi}_1(\mathbf{q},\mathbf{p})| \le \frac{\tilde{c}}{q} \int_0^\infty \frac{dp'}{p'^\epsilon} \, \frac{1}{(p'+p+1)^2} \left(\frac{1}{|q-p'|^\epsilon} - \frac{1}{|q+p'|^\epsilon} \right). \tag{I.2.75}$$

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 $(p'+p+1)^{-2} \le 1$. The resulting integral can be performed analytically with the help of hypergeometric functions (Gradshteyn and Ryzhik 1965, p.284), and it behaves $\sim q^{1-2\epsilon}$ for $q \to 0$. $B_1 V$ is in the same operator class such that we obtain

$$|\hat{w}_2(\mathbf{q},\mathbf{p})| \le c \, \frac{1+q^\epsilon}{q^{2\epsilon}(q+p+1)^2}. \tag{I.2.76}$$

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

Proposition I.2 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 (I.2.55), $\frac{\epsilon}{1-n\epsilon} \delta^{-\frac{1-n\epsilon}{\epsilon}} \to \infty$ as $\epsilon \to 0$, which implies $C \to \infty$ in (I.2.51). Therefore, this limit cannot be used to prove p-form boundedness of V_k, $1 \le k \le n$ with form bound less than one, in the case of the Coulomb potential.

I.3. **Relation to the Douglas-Kroll transformation scheme.**

The Douglas-Kroll transformation scheme for the Dirac operator is based on the Foldy-Wouthuysen (1950) transformation, aimed at casting the free Dirac operator into an operator which does not couple the upper and lower components of the relativistic wavefunction. In this section, the Foldy-Wouthuysen transformation, generalised by Douglas and Kroll (1974) to Dirac operators including an electrostatic potential, will be described. Subsequently, it will be shown that the Douglas-Kroll transformation scheme is equivalent to the Sobolev transformation scheme. Finally, the advantages and drawbacks of the resulting operators will be discussed.

a) The Douglas-Kroll transformation scheme

Like the Sobolev transformation scheme, the Douglas-Kroll transformation scheme consists of a series of unitary operators U_j'. The zeroth-order transformation operator is diagonal in momentum space and is given by

$$U_0' := A(p)\left(1 + \beta \frac{\boldsymbol{\alpha}\mathbf{p}}{E_p + m}\right), \qquad A(p) := \left(\frac{E_p + m}{2E_p}\right)^{\frac{1}{2}}, \tag{I.3.1}$$

and for the transformed Dirac operator one obtains with $U_0'^{-1} = A(p)\,(1 - \beta \frac{\boldsymbol{\alpha}\mathbf{p}}{E_p + m})$

$$\begin{aligned} U_0' H U_0'^{-1} &= \beta E_p + \mathcal{E}_1 + \mathcal{O}_1 \\ \mathcal{E}_1 &:= A(p)\left(V + \frac{\boldsymbol{\alpha}\mathbf{p}}{E_p + m}\, V\, \frac{\boldsymbol{\alpha}\mathbf{p}}{E_p + m}\right) A(p), \\ \mathcal{O}_1 &:= \beta A(p)\left(\frac{\boldsymbol{\alpha}\mathbf{p}}{E_p + m}\, V - V\, \frac{\boldsymbol{\alpha}\mathbf{p}}{E_p + m}\right) A(p). \end{aligned} \tag{I.3.2}$$

When a potential is present the operator $\mathcal{E}_1$, called an even operator because it commutes with β, is also diagonal. But there is an additional term, the so-called odd term $\mathcal{O}_1$ which anticommutes with β and which does couple the two components of ψ. Therefore, the next transformation, U_1', is aimed at eliminating $\mathcal{O}_1$. As has been shown by Wolf, Reiher and Hess (2002), the choice of this transformation is not unique. Historically, a square-root form was chosen, $U_j' = (1 + W_j^2)^{\frac{1}{2}} + W_j,\ j \geq 1$, with antisymmetric operators W_j, i.e. $(\varphi, W_j\varphi) = -(W_j\varphi, \varphi)$. However, in order to establish the equivalence with the Sobolev transformations, an exponential form has to be taken,

$$U_j' := e^{-iS_j}, \qquad j \geq 1, \tag{I.3.3}$$

with essentially self-adjoint operators S_j. For this exponential form, the transformation scheme (I.2.6) from the previous section can be used, such that

$$\begin{aligned} U_1' U_0' \, H \, U_0'^{-1} U_1'^{-1} &= \beta E_p + \mathcal{E}_1 + \mathcal{O}_1 + i[\beta E_p, S_1] + i[\mathcal{E}_1 + \mathcal{O}_1, S_1] \\ &\quad - \frac{1}{2}\,[\,[\beta E_p, S_1],\, S_1] + R(\gamma^3). \end{aligned} \tag{I.3.4}$$

S_1 is chosen as an odd operator which eliminates $\mathcal{O}_1$ according to

$$i\,[\beta E_p, S_j] = -\mathcal{O}_j, \qquad j = 1 \tag{I.3.5}$$

hence S_1 is of first order in the potential like $\mathcal{O}_1$, and the terms which are disregarded in (I.3.4) are in fact at least of third order in the potential. The transformation scheme is continued in the sense that after k transformations, the potential term which is of $k+1$st order in the potential strength, is decomposed into even ($\mathcal{E}_{k+1}$) and odd ($\mathcal{O}_{k+1}$) contributions (corresponding to their behaviour when commuted with β), and the successive transformation $U_{k+1}' = e^{-iS_{k+1}}$ eliminates the odd term by means of the choice (I.3.5) for $j = k+1$. After $n+1$ transformations one arrives at

$$H_n' := \beta E_p + \mathcal{E}_1 + \ldots + \mathcal{E}_n \tag{I.3.6}$$

which only consists of even terms and agrees with the transformed Dirac operator to the order of γ^{n+1}.

With H_n' of this form, one can easily eliminate the lower components of ψ in order to obtain e.g. the nonrelativistic limit. This is either done by choosing $\psi := \binom{u}{0}$, or equivalently, by projecting the block-diagonalised matrix-valued operator H_n' onto the upper block (by means of forming $\frac{1+\beta}{2}\, H_n'\, \frac{1+\beta}{2}$). With this procedure, one has a reduction from the 4-dimensional space of ψ to the 2-dimensional space of u.

Let $\psi := \binom{u}{0}$ with $u \in H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2$ an arbitrary function. Then one can form the expectation value of H_n' and in this way define an operator $b_m^{(n)}$ which acts on

$H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2$ (instead of $H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4$) by means of (Douglas and Kroll 1974, EPS 1996)

$$(\psi, H'_n\, \psi) \;=\; (u, b_m^{(n)}\, u) \tag{I.3.7}$$
$$=\; (u, (b_{0m} \,+\, b_{1m} \,+ ... +\, b_{nm})\, u).$$

The index m refers to the particle mass while the other index denotes the order in the potential strength.

b) Equivalence of Sobolev and Douglas-Kroll transformation scheme

If the Douglas-Kroll unitary transformations are chosen of exponential type, one has a termwise equivalence of the transformed Dirac operator to any order n in the potential strength. For non-exponential unitary transformations, the transformed operator will differ from the Sobolev transformed operator for sufficiently high n (e.g. $n > 4$ for a square-root type). However, the equivalence persists if the same type of unitary transformation (not necessarily exponential) is used in both transformation schemes.

We consider expectation values of the Sobolev transformed Dirac operator taken with a 4-spinor φ in the positive spectral subspace $\mathcal{H}_{+,1} := \Lambda_+(H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4)$ of the free Dirac operator D_0. Such a spinor can in momentum space be expressed in terms of Pauli spinors $u \in H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2$ (Rose 1961, EPS 1996),

$$\hat{\varphi}(\mathbf{p}) \;=\; \frac{1}{\sqrt{2E_p\,(E_p+m)}} \begin{pmatrix} (E_p+m)\;\hat{u}(\mathbf{p}) \\ \mathbf{p}\boldsymbol{\sigma}\;\hat{u}(\mathbf{p}) \end{pmatrix}, \tag{I.3.8}$$

where $\boldsymbol{\sigma}$ is the vector of the three Pauli matrices given in the introduction. We have the following theorem.

Theorem I.2.
Let $\varphi \in \Lambda_+(\mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^4)$ be a 4-spinor in the positive spectral subspace of D_0, which defines a Pauli spinor u according to (I.3.8). Let H'_n be the Douglas-Kroll transformed Dirac operator to n-th order in the potential strength, using exponential unitary operators U'_j. Let $H^{(n)}$ be the Sobolev-transformed operator from Theorem I.1. Then their expectation values agree to any order n,

$$(\varphi, H^{(n)}\,\varphi) \;=\; \left(\varphi, \sum_{k=0}^{n} H_k\,\varphi\right) \;=\; \left(\begin{pmatrix} u \\ 0 \end{pmatrix}, H'_n \begin{pmatrix} u \\ 0 \end{pmatrix}\right) \qquad n = 1, 2, ... \tag{I.3.9}$$

The proof is performed with the help of a lemma.

Lemma I.7 (Relation between transformed potentials).
Let $H \;=\; D_0 + V$ and $U_j \;=\; e^{iB_j}$, $j \;=\; 1, ..., n$ be the Sobolev transformation scheme, where the potential term of k-th order in the potential strength 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 respective decomposition into $\mathcal{E}_k + \mathcal{O}_k$. Then one has the identification

$$\beta E_p \;=\; U'_0\, D_0\, U_0^{'-1}, \qquad \mathcal{E}_k \;=\; U'_0\, V_k\, U_0^{'-1}, \qquad \mathcal{O}_k \;=\; U'_0\, W_k\, U_0^{'-1}$$
$$S_k \;=\; U'_0\, B_k\, U_0^{'-1}, \qquad\qquad k = 1, ..., n \tag{I.3.10}$$

with U'_0 from (I.3.1).

Proof of Theorem.
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,

$$\varphi \;=\; U_0^{'-1}\,\psi, \tag{I.3.11}$$

which is easily verified in momentum space from the explicit form (I.3.8) of $\hat{\varphi}$ and from the definition (I.3.1) of U_0'. We note in passing that $D_0\varphi = E_p\varphi$ is an immediate consequence of (I.3.11).

The first equality of the theorem is based on $\Lambda_+\varphi = \varphi$ and $\Lambda_-\varphi = 0$ such that $(\varphi, V_k\varphi) = (\varphi, (\Lambda_+ H_k \Lambda_+ + \Lambda_- H_k \Lambda_-)\,\varphi) = (\varphi, H_k\varphi)$. Moreover, from $U_0' V_k U_0^{'-1} = \mathcal{E}_k,\;\; k = 1, 2, ...$ and $U_0' D_0 U_0^{'-1} = \beta E_p$ (Lemma I.7), one has

$$(\varphi, H^{(n)}\,\varphi) \;=\; \left(U_0^{'-1}\,\psi, (D_0 + \sum_{k=1}^{n} V_k)\,U_0^{'-1}\,\psi\right) \;=\; \left(\psi, (\beta E_p \,+\, \sum_{k=1}^{n}\mathcal{E}_k)\,\psi\right)$$
$$= \;(\psi, H_n'\,\psi), \tag{I.3.12}$$

which proves the theorem. ■

Proof of Lemma.
We use the induction principle.

(i) Verification of (I.3.10) to first order in γ
The equality $U_0' D_0 U_0^{'-1} = \beta E_p$ follows directly from (I.3.2) if one sets $V = 0$.

By means of explicit calculation, one has from (I.2.18) in the massless ($m = 0$) case

$$U_0'\,W_1\,U_0^{'-1} \;=\; \frac{1}{\sqrt{2}}(1 \,+\, \beta\boldsymbol{\alpha}\hat{\mathbf{p}})\cdot\frac{1}{2}\;(V \;-\; \boldsymbol{\alpha}\;\hat{\mathbf{p}}\;V\;\boldsymbol{\alpha}\hat{\mathbf{p}})\cdot\frac{1}{\sqrt{2}}(1 \,+\, \boldsymbol{\alpha}\hat{\mathbf{p}}\,\beta)$$
$$= \;\frac{1}{2}\;[\beta\,\boldsymbol{\alpha}\hat{\mathbf{p}}\,V \;-\; \beta V\,\boldsymbol{\alpha}\hat{\mathbf{p}}] \;=\; \mathcal{O}_1 \tag{I.3.13}$$

with $\hat{\mathbf{p}} = \mathbf{p}/p$. Similarly, with $V_1 = \frac{1}{2}(V + \boldsymbol{\alpha}\hat{\mathbf{p}}V\boldsymbol{\alpha}\hat{\mathbf{p}})$, one shows $U_0' V_1 U_0^{'-1} = \mathcal{E}_1$. The proof for the massive case proceeds along the same lines, using 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 (I.3.5). Representing S_1 and $\mathcal{O}_1$ by their respective symbols s_1 and o_1 via (I.1.13) and noting that βE_p is a multiplication operator in Fourier space, one obtains from (I.3.5)

$$-\hat{o}_1(\mathbf{q},\mathbf{p}) \;=\; i\beta E_{|\mathbf{p}+\mathbf{q}|}\;\hat{s}_1(\mathbf{q},\mathbf{p}) \;-\; i\hat{s}_1(\mathbf{q},\mathbf{p})\;\beta E_p$$
$$= \;i\beta\left(E_{|\mathbf{p}+\mathbf{q}|} \;+\; E_p\right)\,\hat{s}_1(\mathbf{q},\mathbf{p}) \tag{I.3.14}$$

which can be uniquely solved for $\hat{s}_1(\mathbf{q},\mathbf{p})$. We now transform the defining equation (I.2.10) for B_1 with U_0'

$$U_0'\,W_1\,U_0^{'-1} \;=\; -i\,(U_0' D_0 U_0^{'-1})(U_0' B_1 U_0^{'-1}) \;+\; i\,(U_0' B_1 U_0^{'-1})(U_0' D_0 U_0^{'-1})$$
$$\Longleftrightarrow \qquad \mathcal{O}_1 \;=\; -i\,\left[\beta E_p, U_0' B_1\,U_0^{'-1}\right] \tag{I.3.15}$$

From the uniqueness of the solution it follows from (I.3.15) and (I.3.5) that $U_0' B_1 U_0^{'-1} = S_1$ and hence the uniqueness of the operator B_1.

(ii) Proof for arbitrary order in γ
We assume that to order $n-1$ the claim (I.3.10) of Lemma I.7 holds. As a consequence, the relation between the Dirac operators after $n-1$ transformations (plus the zeroth-order one in the Douglas-Kroll case), asserted by Theorem I.2, does hold too, i.e. (cf. (I.2.11))

$$\beta E_p + \mathcal{E}_1 + \mathcal{E}_2 + ... + \mathcal{E}_{n-1} + \mathcal{E}_n + \mathcal{O}_n = U_0'\;(D_0 + V_1 + ... + V_{n-1} + V_n + W_n)\;U_0^{'-1} \tag{I.3.16}$$

where we are allowed to include the terms of n-th order 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 (I.3.10) for $j = 1, ..., n-1$

it therefore follows that $\mathcal{E}_n = U_0' V_n U_0'^{-1}$ and $\mathcal{O}_n = U_0' W_n U_0'^{-1}$. Carrying out the n-th transformation one gets

$$H_n' = e^{-iS_n} H_{n-1}' e^{iS_n} = \beta E_p + \mathcal{E}_1 + ... + \mathcal{E}_{n-1} + \mathcal{E}_n + \mathcal{O}_n + i\,[\beta E_p, S_n] + R(\gamma^{n+1})$$

$$U_n^+ \cdots U_1^+ \, H \, U_1 \cdots U_n = D_0 + V_1 + ... + V_{n-1} + V_n + W_n + i\,[D_0, B_n] + R(\gamma^{n+1}). \tag{I.3.17}$$

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

$$U_0' \, W_n \, U_0'^{-1} = \mathcal{O}_n = -iU_0' \, [D_0, B_n] \, U_0'^{-1} = -i \, [\beta E_p, U_0' B_n U_0'^{-1}]. \tag{I.3.18}$$

From uniqueness of the solution S_n to the equation $\mathcal{O}_n = -i[\beta E_p, S_n]$ follows $U_0' B_n U_0'^{-1} = S_n$. ■

c) The Jansen-Hess operator representations

The second-order operator H_2' has gained particular attention because, if numerically investigated, its ground-state energy is rather close to the exact solution of the one-particle Dirac equation in the case of a Coulomb potential. In this respect, H_2' is a considerable improvement over the first-order Brown-Ravenhall operator which largely underestimates the ground-state energy for high nuclear charges (Wolf, Reiher and Hess 2002). It was first derived by Jansen and Hess (1989) who added a missing term to the original result of Douglas and Kroll (1974).

(i) The Douglas-Kroll transformed second-order operator

Using the Douglas-Kroll transformation scheme, we define an operator $b_m^{(2)} := b_m := b_{0m} + b_{1m} + b_{2m}$ acting on $H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2$, by virtue of (I.3.7). From their definition, S_k, $\mathcal{E}_k$ and $\mathcal{O}_k$ are integral operators in momentum space, and so are b_{1m}, b_{2m}. However, a coordinate-space representation is sometimes more convenient for the analysis of an operator.

We start from the definition of the Jansen-Hess operator on $H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4$ (Jansen and Hess 1989),

$$H_2' = \beta E_p + \mathcal{E}_1 + \frac{i}{2} \, [\mathcal{O}_1, S_1] \tag{I.3.19}$$

with $\mathcal{E}_1$ and $\mathcal{O}_1$ from (I.3.2) and the symbol of S_1 from (I.3.14). We use $\left(\binom{u}{0}, \alpha_i \alpha_j \binom{u}{0}\right) = (u, \sigma_i \sigma_j u)$ and $\left(\binom{u}{0}, \beta \binom{u}{0}\right) = (u, u)$ as well as $(\boldsymbol{\alpha}\hat{\mathbf{p}})^2 = (\boldsymbol{\sigma}\hat{\mathbf{p}})^2 = 1$, and obtain with $V = -\gamma/x$, identifying $\mathbf{p}$ with $-i\partial/\partial\mathbf{x}$ and p with $(-\Delta)^{\frac{1}{2}}$,

$$b_{0m} = E_p = \sqrt{p^2 + m^2}$$

$$b_{1m} = -\gamma \, A(p) \left[\frac{1}{x} \, A(p) + h(p) \, \boldsymbol{\sigma}\hat{\mathbf{p}} \frac{1}{x} \boldsymbol{\sigma}\hat{\mathbf{p}} \, h(p) \, A(p) \right]$$

$$\begin{aligned} b_{2m} = \left(\frac{\gamma}{2\pi}\right)^2 A(p) \Big[& \frac{1}{x} A^2(p) \, h^2(p) \, W_{10,m} + W_{10,m} A(p) \, h^2(p) \frac{1}{x} A(p) \\ & - \frac{1}{x} A^2(p) \, h(p) \, \boldsymbol{\sigma}\hat{\mathbf{p}} \, W_{11,m} - W_{11,m} A(p) \frac{1}{x} A(p) \, \boldsymbol{\sigma}\hat{\mathbf{p}} \, h(p) \\ & - \boldsymbol{\sigma}\hat{\mathbf{p}} \, h(p) \frac{1}{x} \boldsymbol{\sigma}\hat{\mathbf{p}} \, h(p) \, A^2(p) \, W_{10,m} - \boldsymbol{\sigma}\hat{\mathbf{p}} \, h(p) \, W_{11,m} A(p) \frac{1}{x} A(p) \\ & + \boldsymbol{\sigma}\hat{\mathbf{p}} \, h(p) \frac{1}{x} A^2(p) \, W_{11,m} + \boldsymbol{\sigma}\hat{\mathbf{p}} \, h(p) \, W_{10,m} A(p) \frac{1}{x} A(p) \, \boldsymbol{\sigma}\hat{\mathbf{p}} \, h(p) \Big], \end{aligned} \tag{I.3.20}$$

with $A(p) := \sqrt{\dfrac{E_p + m}{2E_p}}$ and $h(p) := \dfrac{p}{E_p + m}$. For mass $m = 0$, one has $h(p) = 1$ and $A(p) = \frac{1}{\sqrt{2}}$ while in the general case $(m \geq 0)$, $h(p) \in [0, 1]$ and $A(p) \in [\frac{1}{\sqrt{2}}, 1]$

are bounded multiplication operators in momentum space. In the expression for b_{2m} we have introduced (bounded) integral operators $W_{10,m}$ and $W_{11,m}$ which are related to the transformation operator S_1 and are defined in momentum-space representation by means of

$$(\widehat{W_{10,m}\,\varphi})(\mathbf{p}) := \int d\mathbf{p}'\;\frac{1}{|\mathbf{p}-\mathbf{p}'|^2}\;A(p')\;\frac{1}{E_p+E_{p'}}\;\varphi(\mathbf{p}')$$

$$(\widehat{W_{11,m}\,\varphi})(\mathbf{p}) := \int d\mathbf{p}'\;\frac{1}{|\mathbf{p}-\mathbf{p}'|^2}\;\boldsymbol{\sigma}\hat{\mathbf{p}}'\cdot h(p')\;A(p')\;\frac{1}{E_p+E_{p'}}\;\varphi(\mathbf{p}'). \tag{I.3.21}$$

For later use, we also give the Jansen-Hess operator as an integral operator in momentum space. To do so, we Fourier transform the potential $-\gamma/x$, which introduces factors of the type $|\mathbf{p}-\mathbf{p}'|^{-2}$ (see (I.2.19)), and obtain (EPS 1996, BSS 2002)

$$(u, b_m u) = \int d\mathbf{p}\;\overline{\hat{u}(\mathbf{p})}\,b_{0m}(p)\,\hat{u}(\mathbf{p})\;+\int d\mathbf{p}\,d\mathbf{p}'\;\overline{\hat{u}(\mathbf{p})}\,[b_{1m}(\mathbf{p},\mathbf{p}')\;+\;b_{2m}(\mathbf{p},\mathbf{p}')]\,\hat{u}(\mathbf{p}') \tag{I.3.22}$$

where

$$b_{1,m}(\mathbf{p},\mathbf{p}') := -\frac{\gamma}{2\pi^2}\;\frac{1}{|\mathbf{p}-\mathbf{p}'|^2}\;[1\;+\;\boldsymbol{\sigma}\hat{\mathbf{p}}\,\boldsymbol{\sigma}\hat{\mathbf{p}}'\,h(p)\,h(p')]\;A(p)\,A(p')$$

$$b_{2m}(\mathbf{p},\mathbf{p}') := \frac{1}{2}\;\left(\frac{\gamma}{2\pi^2}\right)^2\int d\mathbf{p}''\;\frac{1}{|\mathbf{p}-\mathbf{p}''|^2}\;\frac{1}{|\mathbf{p}''-\mathbf{p}'|^2}\;\left[\frac{1}{E_{p'}+E_{p''}}\;+\;\frac{1}{E_p+E_{p''}}\right]$$

$$\cdot A(p)\,A(p')\,A^2(p'')\;(h(p'')\,\boldsymbol{\sigma}\hat{\mathbf{p}}''\;-\;h(p)\,\boldsymbol{\sigma}\hat{\mathbf{p}})\;(h(p'')\,\boldsymbol{\sigma}\hat{\mathbf{p}}''\;-\;h(p')\,\boldsymbol{\sigma}\hat{\mathbf{p}}'). \tag{I.3.23}$$

Recall that in the momentum representation, the kinetic energy operator $b_{0m}(p) = E_p$ is diagonal. This is of great help when considering the form boundedness and compactness of the potential terms relative to the kinetic energy (see next section).

(ii) The Sobolev transformed second-order operator

Restricting $H_{1/2}(\mathbb{R}^3)\times\mathbb{C}^4$ to the positive spectral subspace of the free Dirac operator, it is sufficient to consider instead of $H^{(2)}$ the operator

$$B_m^{(2)} :=\; D_0\;+\;H_1\;+\;H_2\;=\;D_0\;+\;V\;+\;\frac{i}{2}\,[W_1,B_1] \tag{I.3.24}$$

$$=:\; D_0\;+\;B_{1m}\;+\;B_{2m}$$

which is derived from (I.2.14). For the first term, $i[V_1,B_1]$, from H_2 we have according to Lemma I.7 and (I.3.12), $U_0'\,[V_1,B_1]\,U_0^{'-1}\;=[\mathcal{E}_1,S_1]$. This is an odd operator (because S_1 is odd) and therefore its expectation value formed with $\psi = \binom{u}{0}$ vanishes. So it can be dropped.

The explicit form of the last term, $B_{2m} := \frac{i}{2}\,[W_1,B_1]$ is obtained with the help of the ΨDO technique in a similar way as applied to the calculation of the symbol ϕ_1 of B_1. We use the symbol equation $\hat{j}(\mathbf{q},\mathbf{p})\;=\;\frac{i}{2}\,(\widehat{w_1\phi_1}-\widehat{\phi_1 w_1})(\mathbf{q},\mathbf{p})$ for the symbol j of B_{2m}, together with (I.1.17), and recall that $W_1=\frac{1}{2}(V-\tilde{D}_0V\tilde{D}_0)$ with $\tilde{D}_0$ a multiplier in momentum space. Then we obtain

$$\hat{j}(\mathbf{q},\mathbf{p}) = \frac{i}{4}\;\frac{1}{(2\pi)^{\frac{3}{2}}}\int d\mathbf{p}'\;\Big\{\hat{v}(\mathbf{q}-\mathbf{p}')\hat{\phi}_1(\mathbf{p}',\mathbf{p}) - \tilde{D}_0(\mathbf{q}+\mathbf{p})\,\hat{v}(\mathbf{q}-\mathbf{p}')\,\tilde{D}_0(\mathbf{p}+\mathbf{p}')$$

$$\cdot\hat{\phi}_1(\mathbf{p}',\mathbf{p}) - \hat{\phi}_1(\mathbf{q}-\mathbf{p}',\mathbf{p}+\mathbf{p}')\,\hat{v}(\mathbf{p}') + \hat{\phi}_1(\mathbf{q}-\mathbf{p}',\mathbf{p}+\mathbf{p}')\,\tilde{D}_0(\mathbf{p}'+\mathbf{p})\,\hat{v}(\mathbf{p}')\,\tilde{D}_0(\mathbf{p}')\Big\}. \tag{I.3.25}$$

Alternatively, B_{2m} can be viewed as an integral operator with kernel k_B. There is a simple relation between k_B and the Fourier transform $\hat{j}$ of the symbol of B_{2m}. From (I.1.14) one has

$$\begin{aligned}(\hat{\varphi}, \widehat{B_{2m}\varphi}) &= \int d\mathbf{p}\, \overline{\hat{\varphi}(\mathbf{p})} \int d\mathbf{p}'\, k_B(\mathbf{p},\mathbf{p}')\, \hat{\varphi}(\mathbf{p}') \\ &= \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\mathbf{p}\, \overline{\hat{\varphi}(\mathbf{p})} \int d\mathbf{p}'\, \hat{j}(\mathbf{p}-\mathbf{p}',\mathbf{p}')\, \hat{\varphi}(\mathbf{p}') \\ \Longleftrightarrow \qquad k_B(\mathbf{p},\mathbf{p}') &= \frac{1}{(2\pi)^{\frac{3}{2}}}\, \hat{j}(\mathbf{p}-\mathbf{p}',\mathbf{p}'). \qquad \text{(I.3.26)}\end{aligned}$$

Inserting the expressions (I.2.19) and (I.2.15) for the symbols of V and B_1, respectively, one obtains

$$k_B(\mathbf{p},\mathbf{p}') = \frac{\gamma^2}{16\pi^4} \int d\mathbf{p}'' \frac{1}{|\mathbf{p}''-\mathbf{p}|^2} \frac{1}{|\mathbf{p}''-\mathbf{p}'|^2} (1-\tilde{D}_0(\mathbf{p}''))\left(\frac{1}{E_{p''}+E_p} + \frac{1}{E_{p''}+E_{p'}}\right) \qquad \text{(I.3.27)}$$

where $\tilde{D}_0(\mathbf{p})\, \hat{\varphi}(\mathbf{p}) = \hat{\varphi}(\mathbf{p})$ has been used whenever $\tilde{D}_0$ is acting on φ.

From this kernel, one can derive the coordinate-space representation of B_{2m}. To this aim, we define an auxiliary potential $V_{10,m}$ by means of

$$(\widehat{V_{10,m}\varphi})(\mathbf{p}'') := \int d\mathbf{p}'\, \frac{1}{|\mathbf{p}''-\mathbf{p}'|^2}\, \frac{1}{E_{p''}+E_{p'}}\, \hat{\varphi}(\mathbf{p}'). \qquad \text{(I.3.28)}$$

Then the part of (I.3.27) which is proportional to $(E_{p''}+E_{p'})^{-1}$ leads to the following operator, called J_1,

$$\begin{aligned}(J_1\varphi)(x) &= \frac{\gamma^2}{16\pi^4} \sqrt{\frac{\pi}{2}}\, \frac{1}{x} \int d\mathbf{p}''\, e^{i\mathbf{p}''\mathbf{x}}\, (1-\tilde{D}_0(\mathbf{p}''))\, (\widehat{V_{10,m}\varphi})(\mathbf{p}'') \\ &= \frac{\gamma^2}{8\pi^2}\, \frac{1}{x}\, (1-\tilde{D}_0(\mathbf{p}))\, (V_{10,m}\,\varphi)(\mathbf{x}) \qquad \text{(I.3.29)}\end{aligned}$$

where, as before, $\mathbf{p}$ has to be interpreted as $-i\partial/\partial\mathbf{x}$. The other part of (I.3.27) leads to the conjugate of J_1 (in accordance with the symmetry of B_{2m}). We get

$$B_{2m} = \frac{\gamma^2}{8\pi^2} \left\{ \frac{1}{x}\, (1-\tilde{D}_0(\mathbf{p}))\, V_{10,m} + V_{10,m}\, (1-\tilde{D}_0(\mathbf{p}))\, \frac{1}{x} \right\}. \qquad \text{(I.3.30)}$$

Since $V_{10,m}$ has a very simple structure, it is possible to find its coordinate representation in order to provide an explicit expression for B_{2m}.

We have the identity

$$\frac{1}{E_{p''}+E_{p'}} = \int_0^\infty dt\, e^{-t(E_{p''}+E_{p'})}, \qquad \text{(I.3.31)}$$

leading to a factorisation of the p''- and p'-dependent terms in the integrand. So we obtain

$$V_{10,m} = 2\pi^2 \int_0^\infty dt\, e^{-tE_p}\, \frac{1}{x}\, e^{-tE_p}, \qquad \text{(I.3.32)}$$

resulting in

$$B_{2m} = \frac{\gamma^2}{4} \int_0^\infty dt J(t), \qquad J(t) := C(t)e^{-tE_p} + e^{-tE_p}C(t) \qquad \text{(I.3.33)}$$

where $C(t)$ is a self-adjoint, positive operator,

$$C(t) := \frac{1}{x}\, (1-\tilde{D}_0(\mathbf{p}))\, e^{-tE_p}\, \frac{1}{x}. \qquad \text{(I.3.34)}$$

The latter property is true because one has $(\varphi, (1-\tilde{D}_0)\,\varphi) \;=\; \|\varphi\|^2(1-\frac{(\varphi,\tilde{D}_0\varphi)}{(\varphi,\varphi)}) \;\geq\; \|\varphi\|^2(1-\|\tilde{D}_0\|) \;=0,$ such that $1-\tilde{D}_0 \geq 0$ is a positive operator. From this follows that $(\varphi, C(t)\,\varphi) \;=(e^{-tE_p/2}\,\frac{1}{x}\,\varphi,\;(1-\tilde{D}_0(\mathbf{p}))\;e^{-tE_p/2}\,\frac{1}{x}\,\varphi) \;\geq 0.$

d) Choice of transformation scheme

From a comparison of the Jansen-Hess operator in its representations b_m and $B_m^{(2)}$ in coordinate space, (I.3.20) respective (I.3.24) with (I.3.30), it is obvious that $B_m^{(2)}$, obtained with the Sobolev transformation scheme, has a much simpler shape.

Although we did not find it possible to show positivity of the second-order term B_{2m} from the representation (I.3.33), it is evident from (I.3.27) that its kernel has a positive real part. There is a proof by Iantchenko (see IJA 2003), involving the partial-wave representation of the operator b_{2m} shown in Appendix B, that the respective (partial-wave) kernels of the second-order term of the Jansen-Hess operator are indeed positive.

The breakthrough provided by the Sobolev transformation scheme becomes clear when one proceeds from the one-particle Dirac operator to the multi-particle Coulomb-Dirac operator to be discussed in parts II and III. For example, compare the Douglas-Kroll transformed two-particle second-order operator (Douglas and Kroll 1974, eqs. (4.22) – (4.24)), filling nearly a whole page, with the respective Sobolev transformed operator (II.4.4) which opens the way to mathematical analysis.

The advantage of the Douglas-Kroll transformed operators lies in their ready access to numerical calculations in quantum chemistry (Hess 1986, Wolf, Reiher and Hess 2002,2004). If atomic binding energies and energy shifts due to relativistic processes are of interest, variational calculations are a very efficient tool. Such computations are much simpler if carried out in *two*-dimensional space, permitting an *arbitrary* choice of wavefunction u (without having to care for the restriction to the positive spectral subspace).

I.4. **Boundedness properties and positivity of the Jansen-Hess operator.**

From Theorem I.2, one has the relation between the Douglas-Kroll transformed operator $b_m^{(n)}$ and the Sobolev-transformed operator $B_m^{(n)}$,

$$\begin{pmatrix} b_m^{(n)} & 0 \\ 0 & 0 \end{pmatrix} \;=\; \frac{1}{2}\,(1+\beta)\,U_0'\,B_m^{(n)}\,U_0'^{-1}\,\frac{1}{2}\,(1+\beta) \tag{I.4.1}$$

which differ only by the bounded operators β and U_0'. Therefore, in most cases it plays no role whether the transformed operator is chosen in the form $b_m^{(n)}$ or $B_m^{(n)}$. In the following analysis, both representations will be used.

The boundedness properties of an essentially self-adjoint operator A defined on a dense subset of a Hilbert space $\mathcal{H}$ are crucial for its extension to a self-adjoint operator. Let the operator A consist of the kinetic energy operator D_0 and a sum of potential terms $V_1,...,V_k$. Assume $V_1+...+V_k$ is D_0-form bounded with form bound c less than 1, such that the form domain of A is the same as that of D_0, implying that A is well-defined in the form sense. Then A is form-bounded from below, $(\varphi, A\,\varphi) \;=(\varphi,(D_0+V_1+...+V_k)\,\varphi) \;\geq\; (1-c)\,(\varphi,D_0\varphi) \;>0,$ such that there exists the self-adjoint Friedrichs extension of A on $\mathcal{H}$ (Pearson 1988, p.104; EPS 1996).

a) Collection of literature results

The properties given below concern the Brown-Ravenhall operator $B_m^{(1)},\ b_m^{(1)}$ (EPS 1996, Tix 1997, 1998, Burenkov and Evans 1998) as well as the massless Jansen-Hess operator $b := b^{(2)}$; a few results are also known for the massive Jansen-Hess operator $b_m^{(2)}$ (Stockmeyer 2002, BSS 2002).

Lemma I.8 (Brown-Ravenhall operator)**.**
Let $u \in \mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^2$ *and* $\gamma_{BR} = 2/(\frac{\pi}{2} + \frac{2}{\pi})$.

(i) *Let* $b_m^{(1)} = b_{0m} + b_{1m}$. *Then* b_{1m} *is* b_{0m}*-form bounded with form bound* < 1 *for* $\gamma < \gamma_{BR}$.

(ii) *Let* $b^{(1)} := b_0 + b_1$ *be the massless Brown-Ravenhall operator. Then*

$$|(u,\,(b_{1m}\,-\,b_1)\,u)|\;\le\;\frac{3}{2}\,m\,\gamma\,(u,u). \tag{I.4.2}$$

$$|(u,\,(b_m^{(1)}\,-\,b^{(1)})\,u)|\;\le\;m\,(1+\frac{3}{2}\gamma)\,(u,u).$$

(iii) *For* $\gamma \le \gamma_{BR}$, $b_m^{(1)}$ *is positive. Explicitly,*

$$(u, b_m^{(1)}\,u)\;\ge\;m\,(1-\gamma)\,(u,u). \tag{I.4.3}$$

iv) *In the partial-wave representation of* $b_m^{(1)}$, *the ground-state configuration is* $l = 0,\ s = \frac{1}{2}$.

(v) *If* $\gamma > \gamma_{BR}$, $b_m^{(1)}$ *is unbounded from below.*

The first item of (ii) was proved by Tix (1997), but no explicit bound was given. This was provided later by Stockmeyer (2002). In order to calculate the form bound of the massive Brown-Ravenhall operator relative to the massless one we use the mean value theorem of differential calculus to deduce $0 \le b_{0m} - b_0 = \sqrt{p^2+m^2} - p = m\,(\frac{db_{0m}}{dm})_{m=\mu} = m \cdot \frac{\mu}{\sqrt{p^2+\mu^2}} \le m$ for any number $\mu \in (0,m)$ and all $p \ge 0$. Adding the bound $\frac{3}{2}m\gamma$ of the first-order terms completes the proof.

Positivity was proved by Tix (1998), and items (iv) and (v) were shown by EPS(1996).

In order for $D_0 + V$ to be a well-defined operator in the form sense, V has to be D_0-form bounded with form bound smaller than one (which is the case for $\gamma < \gamma_{BR}$, see EPS(1996) and part II, Lemma II.6).

Lemma I.9 (Positivity of the massless Jansen-Hess operator)**.**
Let $u \in \mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^2$ *and* $\gamma_J = 1.006$ *be the smaller root of* $1 - \frac{\gamma}{\gamma_{BR}} + d\gamma^2 = 0$, $d = \frac{1}{8}(\frac{\pi}{2} - \frac{2}{\pi})^2$.

(i) *Let* $b = b_0 + b_1 + b_2$. *Then* $b_2 \ge 0$.

(ii) *For* $\gamma \le \gamma_J$, *b is positive with*

$$(u, b\,u)\;\ge\;(1\,-\,\frac{\gamma}{\gamma_{BR}}\,+\,d\gamma^2)\,(u, b_0\,u). \tag{I.4.4}$$

(iii) *In the partial-wave representation of b, the ground-state configuration is* $l = 0,\ s = \frac{1}{2}$.

The bound γ_J is not sharp, i.e. b is not unbounded from below for all $\gamma > \gamma_J$ (Siedentop, Priv. Comm.). The reason is that for $\gamma > 9.11$, the r.h.s. of (I.4.4) is again positive.

The proof is performed in Mellin space (Stockmeyer 2002, BSS 2002) which is introduced in Appendix B. When $m \ne 0$, the nonexistent scaling properties of the operator $b_m^{(2)}$ (in contrast to b) prohibit an analogous proof of positivity in the massive case. Instead, one has

Lemma I.10 (Bounds for the massive Jansen-Hess operator)**.**
Let $u \in \mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^2$, *and let* $b_m := b_m^{(2)} = b_{0m} + b_{1m} + b_{2m}$.

(i)
$$|(u,\, (b_{2m} - b_2)\, u)| \;\leq\; m\,\gamma^2 d_0\; (u, u) \tag{I.4.5}$$
with $d_0 := 8 + 12\sqrt{2}$.

(ii)
$$(u, b_m\, u) \;\geq\; d_\gamma\, m\; (u, u) \qquad \textit{for } \gamma \leq \gamma_{BR} \tag{I.4.6}$$
with $d_\gamma := 1 - \gamma - \gamma^2 d$.

(iii)
$$(u, b_m\, u) \;\geq\; -c\, m\; (u, u) \qquad \textit{for } \gamma \leq \gamma_J \tag{I.4.7}$$
and $c := \frac{3}{2}\gamma + d_0\gamma^2$.

The boundedness (ii) from below follows immediately from (I.4.3) and (I.4.5) since $b_2 \geq 0$.

The lower bound (iii) for $\gamma_{BR} < \gamma \leq \gamma_J$ follows from (I.4.2) and (I.4.5) (Stockmeyer 2002).

b) Additional boundedness properties of the Jansen-Hess operator

Our first goal is to show the subordinacy of the second-order term b_{2m} with respect to the first-order term in the potential strength γ.

Proposition I.3 (Subordinacy of b_{2m} respective B_{2m})**.**
Let $B_m^{(2)} = D_0 + B_{1m} + B_{2m}$ *with* $-B_{1m} := -V = \frac{\gamma}{x} \geq 0$. *If* $\gamma \leq 4/\pi$, *then*

(i) *for* $m = 0$,
$$-b_1 \;\geq\; b_2 \;\geq\; 0. \tag{I.4.8}$$

(ii) *For* $m \geq 0$,
$$-B_{1m} \;-\; B_{2m} \;=\; \frac{\gamma}{x}\, R_m \;+\; R_m^*\, \frac{\gamma}{x} \tag{I.4.9}$$
where R_m *is a bounded operator with Re* $R_m \geq 0$.

(iii) *For* $\gamma \leq \frac{4}{\pi C}$, $-B_{1m} - B_{2m}$ *is positive. Explicitly, for* $\varphi \in \Lambda_+(\mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^4)$,
$$(\varphi,\, (-B_{1m} - B_{2m})\, \varphi) \;\geq\; (1 \,-\, C \cdot \frac{\gamma\pi}{4})\; (\varphi, -B_{1m}\, \varphi), \tag{I.4.10}$$
where C *is a constant of order unity.*

The methods of proof for the massless and massive case (i) and (iii), respectively, are very different. For $m = 0$, the proof can be carried out in Mellin space which is a great simplification. For $m \neq 0$, the coordinate-space representation of B_{1m} and B_{2m} has to be used.

Proof of (i).
According to Appendix B, a partial-wave expansion of the function $u \in \mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^2$ in momentum space is made,
$$\hat{u}(\mathbf{p}) \;=\; \sum_\nu p^{-1}\, a_\nu(p)\; \Omega_\nu(\hat{\mathbf{p}}) \qquad\qquad \nu = \{l, M, s\} \tag{I.4.11}$$
and further, the Mellin space representation $a_\nu^\#(t)$ of the coefficient $a_\nu(p)$ is introduced via formula (B.5). The expectation value of b can be written in alternative ways,
$$(\varphi, b\, \varphi) \;=\; \sum_\nu \int_0^\infty dp\; \overline{a_\nu(p)} \int_0^\infty dp'\; b_{ls}(p, p')\; a_\nu(p')$$
$$=\; \sum_\nu \int_{-\infty}^\infty dt\; \left| a_\nu^\#(t + \frac{i}{2}) \right|^2\; b_{ls}^\#(t - \frac{i}{2}) \tag{I.4.12}$$

with b_{ls} and $b_{ls}^{\#}$ given explicitly in (B.4) and (B.7), (B.8), respectively. This shows that b is diagonal in Mellin space. In order to prove $-b_1 - b_2 \geq 0$, it is sufficient to prove

$$-b_{ls}^{(1)\#}(t - \frac{i}{2}) \; - \; b_{ls}^{(2)\#}(t - \frac{i}{2}) \; \geq 0 \tag{I.4.13}$$

where $b_{ls}^{(1)}$ and $b_{ls}^{(2)}$ are the first- and second-order contributions in γ, respectively, to the partial wave b_{ls} of b.

We proceed in two steps. First we show that (I.4.13) holds for any l larger than a given l_1. Subsequently we establish a recurrence relation to prove (I.4.13) inductively for decreasing l.

(α) Search for l_1

The gamma function entering into the definition of $b_{ls}^{(1)\#}$ and $b_{ls}^{(2)\#}$ via (B.9) has the following property (Gradshteyn and Ryzhik 1965, p.937)

$$\lim_{|z|\to\infty} \left| \frac{\Gamma(z+a)}{\Gamma(z)} \; z^{-a} \right|^2 \; = \; 1 \qquad \text{for } z \in \mathbb{C}\backslash(\mathbb{Z}_- \cup \{0\}), \;\; a \in \mathbb{R} \tag{I.4.14}$$

From (B.9) one has $q_l^{\#}(t - \frac{i}{2}) \; = \; \frac{\sqrt{\pi}}{2\sqrt{2}} \; \left| \frac{\Gamma(z+a)}{\Gamma(z)} \right|^2$ for $z := \frac{l}{2} \; + 1 \; - \frac{it}{2}$ and $a := -\frac{1}{2}$. Then (I.4.14) guarantees the existence of $l_0 \in \mathbb{N}$ such that for any ϵ with $0 < \epsilon < 1$, and for all $l > l_0$,

$$(1-\epsilon) \; \frac{1}{\left|\frac{l}{2} + 1 - \frac{it}{2}\right|} \; < \; 2 \, \sqrt{\frac{2}{\pi}} \; q_l^{\#}(t - \frac{i}{2}) \; < \; (1+\epsilon) \; \frac{1}{\left|\frac{l}{2} + 1 - \frac{it}{2}\right|}. \tag{I.4.15}$$

From this and from the functional dependence (B.8) of $b_{ls}^{(1)\#}$ and $b_{ls}^{(2)\#}$ on $q_l^{\#}$ it follows that the upper and lower bounds of $q_l^{\#}(t - i/2)$ and hence of $b_{ls}^{(1)\#}(t - i/2)$ decrease as l^{-1} for $l \to \infty$, while the bounds of $b_{ls}^{(2)\#}(t - i/2)$ are of order $O(l^{-2})$ making that term negligible with respect to $b_{ls}^{(1)\#}(t - i/2)$ for sufficiently large l. Since $-b_{ls}^{(1)\#}(t - \frac{i}{2})$ is strictly positive for $\gamma > 0$, it follows that there exists $l_1 \in \mathbb{N}$ such that

$$(-b_{ls}^{(1)\#} \; - b_{ls}^{(2)\#})(t - \frac{i}{2}) \; \geq 0 \qquad \text{for all } l \geq l_1, \; s = \pm\frac{1}{2}. \tag{I.4.16}$$

(β) Recurrence relation

From the explicit representation (B.8) one has $b_{l+1,-\frac{1}{2}}^{(i)\#}(t - \frac{i}{2}) \; = b_{l,\frac{1}{2}}^{(i)\#}(t - \frac{i}{2})$, $i = 1, 2, \;\; l \in \mathbb{N}_0$, such that we can restrict ourselves to $s = \frac{1}{2}$.

For $\gamma \leq 4/\pi$ it was shown by Stockmeyer (2002) and BSS (2002) that

$$1 \, + \, \sqrt{2\pi} \, (b_{l,1/2}^{(1)\#} \, + \, b_{l,1/2}^{(2)\#})(t - \frac{i}{2}) \; \leq \; 1 \, + \, \sqrt{2\pi} \, (b_{l+1,1/2}^{(1)\#} \, + \, b_{l+1,1/2}^{(2)\#})(t - \frac{i}{2}). \tag{I.4.17}$$

Hence

$$(-b_{l+1,s}^{(1)\#} - b_{l+1,s}^{(2)\#})(t - \frac{i}{2}) \leq (-b_{ls}^{(1)\#} - b_{ls}^{(2)\#})(t - \frac{i}{2}), \quad (l,s) \in \{(\mathbb{N}_0, \frac{1}{2}) \cup (\mathbb{N}, -\frac{1}{2})\}. \tag{I.4.18}$$

Starting in the r.h.s. of (I.4.18) with $l = 0$ if $s = \frac{1}{2}$ and with $l = 1$ for $s = -\frac{1}{2}$ and continuing the chain of inequalities to the left until l_1 is reached, proves that $(-b_{ls}^{(1)\#} - b_{ls}^{(2)\#})(t - i/2) \; \geq 0$ for all l, s. ∎

Proof of (ii).

From the Sobolev representation (I.3.24) with (I.3.30) we have, using $\Lambda_- =$

$(1 - \tilde{D}_0(\mathbf{p}))/2$,

$$-(B_{1m} + B_{2m}) \;=\; \frac{\gamma}{x}\, R_m \;+\; R_m^* \,\frac{\gamma}{x} \tag{I.4.19}$$

$$R_m := \;\frac{1}{2} \;-\; \frac{\gamma}{4\pi^2}\,\Lambda_-\, V_{10,m}.$$

We prove that R_m is bounded with positive real part if $\gamma \le \frac{4}{\pi}$, by showing that $\|\frac{\gamma}{4\pi^2}\,\Lambda_-\, V_{10,m}\| \;\le \frac{1}{2}$, i.e. for $\varphi \in L_2(\mathbb{R}^3) \times \mathbb{C}^4$,

$$\|\frac{\gamma}{4\pi^2}\,\Lambda_-\, V_{10,m}\,\varphi\| \;\le\; \frac{\gamma}{4\pi^2}\,\|\Lambda_-\|\,\|V_{10,m}\,\varphi\| \;\le\; \frac{\gamma}{4\pi^2}\,\|\Lambda_-\|\,\|V_{10,m}\|\cdot\|\varphi\| \;\le\; c\,\|\varphi\| \tag{I.4.20}$$

with $c \le \frac{1}{2}$. Note that $\|\Lambda_-\| = 1$, and that the adjoint operator is also estimated by the r.h.s. of (I.4.20).

Because of Lemma I.3 it is sufficient to prove the above boundedness for the quadratic form of $V_{10,m}$. Using the momentum representation (I.3.28) and the Lieb and Yau formula, Lemma I.1, one has

$$|(\varphi, V_{10,m}\,\varphi)| \;=\; \int d\mathbf{p}\;\overline{\hat{\varphi}(\mathbf{p})}\int d\mathbf{p}'\;\frac{1}{|\mathbf{p}-\mathbf{p}'|^2}\;\frac{1}{E_p + E_{p'}}\;\hat{\varphi}(\mathbf{p}')$$

$$\le\; \int d\mathbf{p}\;|\hat{\varphi}(\mathbf{p})|^2\int d\mathbf{p}'\;\frac{1}{|\mathbf{p}-\mathbf{p}'|^2}\;\frac{1}{p+p'}\;\frac{f(p)}{f(p')} \tag{I.4.21}$$

where the estimate $E_p \ge p$ was used. Choosing $f(p) = p$ one obtains with Appendix A,

$$|(\varphi, V_{10,m}\,\varphi)| \;\le\; \int d\mathbf{p}\;|\hat{\varphi}(\mathbf{p})|^2\cdot\frac{\pi^3}{2} \tag{I.4.22}$$

and consequently from Lemma I.3, $\|V_{10,m}\,\varphi\| \;\le\; \frac{\pi^3}{2}\,\|\varphi\|$. In order to restrict the constant c in (I.4.20) to $\frac{1}{2}$, one needs $\frac{\gamma}{4\pi^2}\cdot\frac{\pi^3}{2} \;\le \frac{1}{2}$. which leads to the condition $\gamma \le \frac{4}{\pi}$. ■

Proof of (iii).
For boundedness proofs of an operator B relative to an operator A a diagonal representation of the dominating operator A is of advantage. Should B be nondiagonal in this representation, it can nevertheless be estimated (by means of the Lieb and Yau formula) by a diagonal operator which is in the same symbol class as B. In the present case, the operator A stands for the Coulomb field V which is diagonal in coordinate space. Therefore, the kernel k_B of the subordinate second-order operator B_{2m} is required in coordinate space.

We use the inverse Fourier transform, $\hat{\varphi}(\mathbf{p}) \;=\; \frac{1}{(2\pi)^{3/2}}\int d\mathbf{x}\, e^{-i\mathbf{p}\mathbf{x}}\,\varphi(\mathbf{x})$, to cast (I.3.26) into the form

$$(\varphi, B_{2m}\,\varphi) \;=\; \int d\mathbf{x}\;\overline{\varphi(\mathbf{x})}\int d\mathbf{x}'\;k(\mathbf{x},\mathbf{x}')\;\varphi(\mathbf{x}') \tag{I.4.23}$$

$$k(\mathbf{x},\mathbf{x}') := \;\frac{1}{(2\pi)^3}\int d\mathbf{p}\;e^{i\mathbf{p}\mathbf{x}}\int d\mathbf{p}'\;k_B(\mathbf{p},\mathbf{p}')\;e^{-i\mathbf{p}'\mathbf{x}'}.$$

Then we can estimate with Lemma I.1

$$-(\varphi,\,(B_{1m} + B_{2m})\,\varphi) \;\ge\; -(\varphi, B_{1m}\,\varphi) \;-\; |(\varphi, B_{2m}\,\varphi)|$$

$$\ge\; -(\varphi, B_{1m}\,\varphi) \;-\; \int d\mathbf{x}\;|\varphi(\mathbf{x})|^2\int d\mathbf{x}'\;|k(\mathbf{x},\mathbf{x}')|\;\frac{f(x)}{f(x')}. \tag{I.4.24}$$

In Appendix E it is shown that the second integral can be estimated by $C \cdot \frac{\pi\gamma^2}{4}\,\frac{1}{x}$ with some constant C. Thus,

$$-(\varphi,\,(B_{1m}+B_{2m})\,\varphi)\;\geq\;\int d\mathbf{x}\;|\varphi(\mathbf{x})|^2\;\frac{\gamma}{x}\;\Big(1\,-\,C\cdot\frac{\gamma\pi}{4}\Big)\,, \tag{I.4.25}$$

from which it follows that $-B_{1m}-B_{2m}\geq 0$ for $\gamma\leq\frac{4}{\pi C}$. On the other hand, we have the estimate (I.4.8) for the massless case, which provides the sharp critical potential strength $\gamma=\frac{4}{\pi}$ for positivity of $-b_1-b_2$. Upon comparing with (I.4.25) which holds for $m\geq 0$, we conjecture that we can set $C=1$. The strict proof for $C=1$ would require a numerical computation of the integrals in (E.3). ■

As a consequence of Proposition I.3, we get form boundeness of the second-order potential term relative to the first-order term. From (I.4.10) and (I.4.24) we have for all $m\geq 0$

Corollary.

$$|\,(\varphi,B_{2m}\,\varphi)|\;\leq\;C\;\frac{\gamma\pi}{4}\;(\varphi,-B_{1m}\,\varphi) \tag{I.4.26}$$

with form bound <1 for $\gamma<4/\pi C$.

Now we turn to the form boundedness of the total potential relative to the kinetic energy. For subcritical potential strength where the form bound is less than one, the Jansen-Hess operator is well-defined in the form sense and, thanks to its boundedness from below, (I.4.7), its Friedrichs extension exists to a self-adjoint operator on $L_2(\mathbb{R}^3)\times\mathbb{C}^2$ respective $\Lambda_+(L_2(\mathbb{R}^3)\times\mathbb{C}^4)$.

Proposition I.4 ($|D_0|$-form boundedness of total potential)**.**
Let $b_m=b_{0m}+b_{1m}+b_{2m}$ be the Jansen-Hess operator and let $u\in H_{1/2}(\mathbb{R}^3)\times\mathbb{C}^2$. Then for all masses $m\geq 0$ we have

$$|(u,\,(b_{1m}+b_{2m})\,u)|\;\leq\;c\,(u,b_{0m}\,u)\;+\;C\,(u,u) \tag{I.4.27}$$

with $c<1$ for $\gamma<\gamma_J=1.006$, and $C\in\mathbb{R}$. For $m=0$ we have $C=0$.

Proof.
Let first $m=0$. From Lemma I.9 we have

$$(u,b\,u)\;\geq\;\epsilon\,(u,b_0\,u) \tag{I.4.28}$$

with $0<\epsilon<1$ for $0<\gamma<\gamma_J$. Inserting $b=b_0+b_1+b_2$ leads with Proposition I.3 to

$$0\;\leq\;(u,\,(-b_1-b_2)\,u)\;\leq\;(1-\epsilon)\,(u,b_0\,u) \tag{I.4.29}$$

which proves (I.4.27) with $C=0$.

For $m\neq 0$ we estimate

$$|(u,\,(b_{1m}+b_{2m})\,u)|\;\leq\;|(u,\,(b_{1m}-b_1)\,u)|\;+\;|(u,\,(b_{2m}-b_2)\,u)|\;+\;|(u,\,(b_1+b_2)\,u)|. \tag{I.4.30}$$

The first two terms are estimated by constants with the help of Lemmata I.8 and I.10, while the b_0-form boundedness of the last (massless) term has just been proved. Collecting results and using that $0\leq b_0\leq b_{0m}$,

$$|(u,\,(b_{1m}+b_{2m})\,u)|\;\leq\;\frac{3}{2}m\gamma\,(u,u)\;+\;m\gamma^2 d_0\,(u,u)\;+\;(1-\epsilon)\,(u,b_0\,u)$$

$$\leq\;m\,(\frac{3}{2}\gamma\;+\;\gamma^2 d_0)\,(u,u)\;+\;(1-\epsilon)\,(u,b_{0m}\,u) \tag{I.4.31}$$

which completes the proof of (I.4.27). ■

c) Positivity of the massive Jansen-Hess operator

Whereas positivity of the massless Jansen-Hess operator is established for all potential strengths up to γ_J (Lemma I.9) we were not able to reach this ambitious goal for $m \neq 0$. Using positivity of the kernel k_B of the (second-order) Jansen-Hess term B_{2m} we have, however,

Proposition I.5 (Positivity of b_m for $m \neq 0$)**.**
Let $b_m = b_{0m} + b_{1m} + b_{2m}$ be the Jansen-Hess operator acting on $H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2$. Then $b_m > 0$ for $\gamma < \gamma_c$, explicitly

$$(u, b_m\, u) \;\geq\; c(\gamma)\; (u, b_{0m}\, u) \tag{I.4.32}$$

with $c(\gamma) > 0$ for $\gamma < \gamma_c = 0.5929$ $(Z \leq 81)$. In case the proof is carried out numerically, the critical coupling strength is increased to $\tilde{\gamma}_c = 0.8368$ $(Z \leq 114)$. $c(\gamma)$ is equal to $\inf\limits_{x \in \mathbb{R}_+} G_{0\frac{1}{2}}(x)$ from (I.4.48) and (I.4.53), respectively.

We note that from the partial-wave decomposition (B.3) of the expectation value of b_m it follows that b_m is positive if the components b_{lsm} associated with each partial wave $\nu = \{l, M, s\}$ are positive.

For the proof a lemma is needed, stating that the largest kernel of the family b_{lsm} is supplied by the lowest angular momentum channel.

Lemma I.11 (Monotonicity of the kernel $b_{lsm}(p,p')$)**.**
Let $b_{lsm}(p,p') \;=\; b_{0m}(p)\,\delta(p-p') \,+\, b^{(1)}_{lsm}(p,p') \,+\, b^{(2)}_{lsm}(p,p')$ be the kernel of the partial-wave decomposed Jansen-Hess operator in momentum space, acting on $H_{1/2}(\mathbb{R}_+ \cup \{0\})$. For all $p, p' \geq 0$, $l \in \mathbb{N}_0$ we have

(i)

$$-b^{(1)}_{lsm}(p,p') \;\leq\; -b^{(1)}_{0\frac{1}{2}m}(p,p') \qquad \text{for } s = \pm\frac{1}{2} \tag{I.4.33}$$

(ii)

$$b^{(2)}_{lsm}(p,p') \;\leq\; b^{(2)}_{0\frac{1}{2}m}(p,p') \qquad \text{for } s = \frac{1}{2},\;\; l \geq 0 \tag{I.4.34}$$

$$b^{(2)}_{lsm}(p,p') \;\leq\; b^{(2)}_{1-\frac{1}{2}m}(p,p') \qquad \text{for } s = -\frac{1}{2},\;\; l \geq 1.$$

The Brown-Ravenhall case (i), proved by EPS (1996), follows immediately from the explicit form of $b^{(1)}_{lsm}(p,p')$ given in (B.3), since the reduced Legendre functions $q_l(y)$ are monotonically decreasing in l for all $y \neq 1$. The estimates (ii) for the second-order terms were proved by Iantchenko (see IJA 2003).

Corollary.
For $m \neq 0$, the ground-state configuration in the partial-wave representation of b_m is a superposition of $l = 0, s = \frac{1}{2}$ and $l = 1, s = -\frac{1}{2}$ components.

As concerns the missing link in (ii), the dominance of $b^{(2)}_{0\frac{1}{2}m}(p,p')$ over $b^{(2)}_{1-\frac{1}{2}m}(p,p')$, we note that for $m \neq 0$, the kernels scale with m,

$$b^{(k)}_{lsm}(p,p') \;=\; b^{(k)}_{ls1}(q,q') \qquad k = 1, 2, \tag{I.4.35}$$

where $q := p/m$, $q' := p'/m$, and for $k = 2$, $q'' := p''/m$ have to be substituted in the expressions (B.3). Hence with $p, p' \in [0, \infty)$, one also has $q, q' \in [0, \infty)$, such that one can restrict oneself to the case $m = 1$. We have numerical evidence that indeed, $b^{(2)}_{0\frac{1}{2}1}(p,p') - b^{(2)}_{1-\frac{1}{2}1}(p,p') \geq 0$ for all $p, p' \geq 0$. Note, however, that there is no global dominance of the *integrand* in $b^{(2)}_{lsm}(p,p')$ for $l = 0$ over the one for $l = 1$. This is to be contrasted to the proof of Lemma I.11(ii) which profits from the global dominance of the integrand for the minimum l considered.

Proof of Proposition.
Consider the estimate of the energy in a partial-wave state a_ν, defined by (B.1) and (B.3),

$$\begin{aligned}(a_\nu, b_{lsm}\, a_\nu) \;&\geq\; (a_\nu, b_{0m}\, a_\nu) \;+\; (a_\nu, b^{(1)}_{lsm}\, a_\nu) \;-\; |(a_\nu, b^{(2)}_{lsm}\, a_\nu)| \\ &\geq\; (a_\nu, b_{0m}\, a_\nu) \;-\; (|a_\nu|, -b^{(1)}_{lsm}\, |a_\nu|\,) \;-\; (|a_\nu|, b^{(2)}_{lsm}\, |a_\nu|\,) \qquad \text{(I.4.36)}\end{aligned}$$

where we have used that the kernels of $-b^{(1)}_{lsm}$ and $b^{(2)}_{lsm}$ are positive (cf. (B.3) and IJA 2003). The last two terms can be estimated with the help of the Lieb and Yau formula of Lemma I.1.

Consider first the case $s = \frac{1}{2}$. Following EPS(1996), the first-order term with its explicit form (B.3) is estimated by

$$\int_0^\infty \int_0^\infty dp\, dp'\; |a_\nu(p)| \; - b^{(1)}_{lsm}(p, p')\; |a_\nu(p')| \qquad \text{(I.4.37)}$$

$$\leq \frac{\gamma}{\pi} \int_0^\infty dp\; |a_\nu(p)|^2\; A^2(p)\; \left\{ \int_0^\infty dp'\; q_l(\frac{p}{p'})\; \frac{p}{p'} \;+ h^2(p) \int_0^\infty dp'\; q_{l+2s}(\frac{p}{p'})\; \frac{p}{p'} \right\}$$

where here and in the following we use $f(p) = p$ for the convergence generating function. Using that $q_l(y)$ is monotonically decreasing in l we obtain with the formulae from Appendix A

$$\begin{aligned}\int_0^\infty dp' \left[q_l(\frac{p}{p'}) \;+ h^2(p)\; q_{l+1}(\frac{p}{p'}) \right] \frac{p}{p'} \;&\leq\; \int_0^\infty dp' \left[q_0(\frac{p}{p'}) \;+ h^2(p)\; q_1(\frac{p}{p'}) \right] \frac{p}{p'} \\ &=\; p\, \left(\frac{\pi^2}{2} \;+\; 2\, h^2(p) \right). \qquad \text{(I.4.38)}\end{aligned}$$

For the second-order term in (I.4.36) we make the additional estimates

$$A^2(p'') \left(\frac{1}{E_{p'} + E_{p''}} \;+\; \frac{1}{E_p + E_{p''}} \right) \;\leq\; \frac{E_{p''} + m}{2E_{p''}} \cdot \frac{2}{m + E_{p''}} \;\leq\; \frac{1}{p''}, \qquad \text{(I.4.39)}$$

and we also drop the two negative terms in the integrand of the kernel of $b^{(2)}_{lsm}$. Then we get

$$\begin{aligned}(\,|a_\nu|, b^{(2)}_{lsm}\, |a_\nu|\,) \;\leq\; &\frac{\gamma^2}{2\pi^2} \int_0^\infty dp\; |a_\nu(p)|^2\; A(p)^2 \int dp'\; \frac{p}{p'} \int_0^\infty \frac{dp''}{p''} \\ &\cdot \left\{ q_l(\frac{p''}{p})\; q_l(\frac{p''}{p'})\; h^2(p'') \;+\; h^2(p)\; q_{l+1}(\frac{p''}{p})\; q_{l+1}(\frac{p''}{p'}) \right\}. \qquad \text{(I.4.40)}\end{aligned}$$

We estimate the integrand again by its value at $l = 0$ and use that $h^2(p'') \leq 1$. We substitute $z := p'/p''$ for p'. Then, the integrals decouple and one gets with Appendix *A*

$$\begin{aligned}\int_0^\infty dp'\; \frac{p}{p'} \int_0^\infty \frac{dp''}{p''}\; q_l(\frac{p''}{p}) q_l(\frac{p''}{p'})\; h^2(p'') \;&\leq\; \int_0^\infty \frac{dp''}{p''}\; q_0(\frac{p''}{p}) \int_0^\infty dp'\; \frac{p}{p'}\; q_0(\frac{p''}{p'}) \\ &=\; p \int_0^\infty \frac{dp''}{p''}\; q_0(\frac{p''}{p}) \cdot \int_0^\infty \frac{dz}{z}\; q_0(z) \;=\; p\, \left(\frac{\pi^2}{2} \right)^2, \qquad \text{(I.4.41)}\end{aligned}$$

and similarly for the second term,

$$\int_0^\infty dp'\; \frac{p}{p'} \int_0^\infty \frac{dp''}{p''}\; q_{l+1}(\frac{p''}{p})\; q_{l+1}(\frac{p''}{p'}) \;\leq p \int_0^\infty \frac{dp''}{p''}\; q_1(\frac{p''}{p}) \cdot \int_0^\infty \frac{dz}{z}\; q_1(z) \;=\; p \cdot 2^2. \qquad \text{(I.4.42)}$$

Collecting results, the expectation value of the Jansen-Hess operator is estimated by

$$(a_\nu, b_{l\frac{1}{2}m} a_\nu) \;\geq \int_0^\infty dp\; |a_\nu(p)|^2\; E_p \cdot G_{0\frac{1}{2}}(p), \qquad \text{(I.4.43)}$$

$$G_{0\frac{1}{2}}(p) := 1 - \frac{\gamma}{\pi}\frac{p}{E_p}A^2(p)\left(\frac{\pi^2}{2} + 2h^2(p)\right) - \frac{\gamma^2}{2\pi^2}\frac{p}{E_p}A^2(p)\left(\frac{\pi^4}{4} + 4h^2(p)\right).$$

The m-invariance of $G_{0\frac{1}{2}}(p)$ for $m \neq 0$ becomes obvious when $x := p/m$ is introduced. Then $E_p = m\sqrt{x^2+1}$ and with the definitions of $A(p)$ and $h(p)$ (given below (I.3.20)) one has

$$G_{0\frac{1}{2}}(mx) = 1 - \frac{\gamma}{\pi}x\left\{\frac{\sqrt{x^2+1}+1}{x^2+1}\left(\frac{\pi^2}{4} + \frac{\gamma\pi^3}{16}\right) + \frac{x^2}{(\sqrt{x^2+1}+1)(x^2+1)}\left(1+\frac{\gamma}{\pi}\right)\right\} \tag{I.4.44}$$

which is independent of m. Hence, $G_{0\frac{1}{2}}(mx) = G_{0\frac{1}{2}}(x)$.

If $G_{0\frac{1}{2}}(x) > 0$ then $b_{l\frac{1}{2}m} > 0$. One easily derives $G_{0\frac{1}{2}}(x) = 1$ for $x = 0$ and $G_{0\frac{1}{2}}(x) \to 1 - \frac{\gamma}{\pi}(1 + \frac{\pi^2}{4} + \frac{\gamma}{\pi} + \gamma\frac{\pi^3}{16})$ for $x \to \infty$ which is positive for sufficiently small γ. Our strategy is to look for $\min_{x\in\mathbb{R}_+} G_{0\frac{1}{2}}(x)$ as a function of γ and subsequently determine γ_c by requiring that this minimum is zero.

The requirement $G'_{0\frac{1}{2}}(x) = 0$ gives the following equation for the minimum value x_0

$$\alpha x_0^2 = \alpha\,(1+\sqrt{x_0^2+1}\,) + \beta\,\frac{3x_0^2\sqrt{x_0^2+1} + x_0^4 + 3x_0^2}{(\sqrt{x_0^2+1}+1)^2} \tag{I.4.45}$$

with $\alpha := \frac{\pi^2}{4} + \frac{\gamma\pi^3}{16}$ and $\beta := 1 + \frac{\gamma}{\pi}$. Defining $z_0 := \sqrt{x_0^2+1}$ this results in a quadratic equation for z_0,

$$(z_0 - 2)\,(z_0+1)\,\alpha = \beta\,(z_0-1)\,(z_0+2) \tag{I.4.46}$$

with the solution (since $z_0 \geq 1$ and $\alpha > \beta$)

$$z_0 = \frac{\alpha + \beta + \sqrt{9\alpha^2 + 9\beta^2 - 14\alpha\beta}}{2(\alpha-\beta)}. \tag{I.4.47}$$

From this one can calculate

$$G_{0\frac{1}{2}}(x_0) = 1 - \frac{\gamma}{\pi}x_0\frac{1}{z_0^2}\left[\alpha\,(z_0+1) + \beta\,(z_0-1)\right] \overset{!}{=} 0 \tag{I.4.48}$$

resulting in $\gamma_c = 0.5929$.

Now we turn to the case $s = -\frac{1}{2}$. For these states, one can again use $q_{l-1}(y) \leq q_0(y)$ to estimate the expectation values of $b^{(1)}_{lsm}$ and $b^{(2)}_{lsm}$ by those for $l = 1$ and $s = -\frac{1}{2}$. The subsequent method of calculation is the same as for the states with $l = 0,\ s = \frac{1}{2}$, only that $q_0(y)$ and $q_1(y)$ are interchanged. Instead of (I.4.43) one now obtains

$$(a_\nu, b_{l-\frac{1}{2}m}a_\nu) \geq \int_0^\infty dp\,|a_\nu(p)|^2\,E_p\cdot G_{1-\frac{1}{2}}(p), \tag{I.4.49}$$

$$G_{1-\frac{1}{2}}(p) := 1 - \frac{\gamma}{\pi}\frac{p}{E_p}A^2(p)\left(2 + \frac{\pi^2}{2}h^2(p)\right) - \frac{\gamma^2}{2\pi^2}\frac{p}{E_p}A^2(p)\left(4 + \frac{\pi^4}{4}h^2(p)\right).$$

We will show that (with $p := mx$)

$$G_{1-\frac{1}{2}}(x) = 1 - \frac{\gamma}{\pi}x\left\{\frac{\sqrt{x^2+1}+1}{x^2+1}(1+\frac{\gamma}{\pi}) + \frac{\sqrt{x^2+1}-1}{x^2+1}(\frac{\pi^2}{4} + \frac{\gamma\pi^3}{16})\right\} \tag{I.4.50}$$

is monotonically decreasing, attaining its infimum at $x \to \infty$, namely $G_{1-\frac{1}{2}}(x) \to 1 - \frac{\gamma}{\pi}(1 + \frac{\pi^2}{4}) - \frac{\gamma^2}{\pi^2}(1 + \frac{\pi^4}{16})$. This limit value is again strictly decreasing with γ, and at $\gamma = \gamma_c = 0.5929$, it equals $0.0932 > 0$. This shows that $(a_\nu, b_{l,-\frac{1}{2},m}a_\nu) > 0$ for $\gamma \leq \gamma_c$ such that we have finally proved $(a_\nu, b_{lsm}a_\nu) > 0$ for $\gamma < \gamma_c$.

The derivative of $G_{1-\frac{1}{2}}(x)$ can be cast into the form

$$-G'_{1-\frac{1}{2}}(x) \;=\; \frac{\gamma}{\pi}\frac{1}{(x^2+1)^2}\left\{x^2\left(\frac{\pi^2}{4}-1\right)+\sqrt{x^2+1}\left(1+\frac{\pi^2}{4}\right)+1-\frac{\pi^2}{4}\right.$$

$$\left.+\;\gamma\left[x^2\left(\frac{\pi^3}{16}-\frac{1}{\pi}\right)+\sqrt{x^2+1}\left(\frac{1}{\pi}+\frac{\pi^3}{16}\right)+\frac{1}{\pi}-\frac{\pi^3}{16}\right]\right\} \ldots\ldots \qquad \text{(I.4.51)}$$

The r.h.s. of (I.4.51) is positive for all $x \in \mathbb{R}_+$ since $\sqrt{x^2+1} \geq 1$, showing that $G_{1-\frac{1}{2}}(x)$ is monotonically decreasing.

The critical potential strength can be improved by evaluating numerically the integrals over the kernel of $b^{(2)}_{lsm}$ which result from the Lieb and Yau formula, without any further estimate. For the Brown-Ravenhall operator an improved estimate for $s=\frac{1}{2}$, provided by Tix(1998), is used,

$$(a_\nu, (b_{0m} + b^{(1)}_{lsm})\, a_\nu) \;\geq\; \int_0^\infty dp\; |a_\nu(p)|^2\; E_p\; T_{0\frac{1}{2}}(x), \qquad \text{(I.4.52)}$$

$$T_{0\frac{1}{2}}(x) := \;1\;-\frac{\gamma}{2}\left\{(\sqrt{x^2+1}+1)\;\frac{\arctan x}{x}\;+\;\frac{(\sqrt{x^2+1}-1)(x-\arctan x)}{(x^2+1)\;\arctan x - x}\right\},$$

valid for all l, s according to EPS(1996).

Then, estimates for the expectation values of $b_{l\frac{1}{2}m}$ and $b_{l-\frac{1}{2}m}$ similar to those given in (I.4.43) and (I.4.49) result, with the functions $G_{0\frac{1}{2}}(x)$ and $G_{1-\frac{1}{2}}(x)$ replaced by new functions $\tilde{G}_{0\frac{1}{2}}(x)$ and $\tilde{G}_{1-\frac{1}{2}}(x)$, respectively. One can show numerically that $\tilde{G}_{0\frac{1}{2}}(x)$ is monotonically decreasing in x, attaining its infimum at $x \to \infty$,

$$\inf_{x\in\mathbb{R}_+} \tilde{G}_{0\frac{1}{2}}(x) \;=\; 1\;-\;\frac{\gamma}{2}\left(\frac{\pi}{2}+\frac{2}{\pi}\right)\;-\;\frac{\gamma^2}{8}\left(\frac{\pi}{2}-\frac{2}{\pi}\right)^2. \qquad \text{(I.4.53)}$$

From setting this equal to zero, the value $\tilde{\gamma}_c = 0.8368$ is obtained.

For the case $s=-\frac{1}{2}$ $(l \geq 1)$, the first-order term is also evaluated numerically without any further approximation, and the factor $h(p)h(p')$ is kept in the kernel when applying the Lieb and Yau formula. Then it is found (numerically) that $\tilde{G}_{1-\frac{1}{2}}(x)$ is monotonically decreasing with its infimum at $x=\infty$ again given by (I.4.53). Moreover, one always has $\tilde{G}_{1-\frac{1}{2}}(x) > \tilde{G}_{0\frac{1}{2}}(x)$. Thus $\tilde{G}_{1-\frac{1}{2}}(x) > 0$ if $\gamma < \tilde{\gamma}_c$.

Collecting results, we have $b_{lsm} > 0$ for $s = \pm\frac{1}{2}$ and $\gamma < \tilde{\gamma}_c$. ■

The present proof of positivity by means of the Lieb and Yau formula cannot be extended to provide critical potential strengths beyond $\tilde{\gamma}_c$. This is lower than the Brown-Ravenhall value, $\gamma_{BR} = 0.906$ $(Z \leq 124$; EPS 1996), derived from (I.4.53) by dropping the quadratic term in γ.

One might think of a different way to prove positivity of b_m, by trying to establish that $-b^{(1)}_{lsm}(p,p') > b^{(2)}_{lsm}(p,p')$ for all values of p, p' and subsequently using the method of proof of Lemma 1 in EPS (1996). In Appendix G it is shown, however, that there is some region of p, p' where $b^{(2)}_{lsm}(p,p')$ is dominating.

I.5. **Spectral properties of the Jansen-Hess operator.**

The spectrum σ of a self-adjoint operator (which in our case is the Friedrichs extension on the Hilbert space $L_2(\mathbb{R}^3)\times\mathbb{C}^2$) consists of the essential spectrum σ_{ess} and the eigenvalues of finite multiplicity. The essential spectrum, in turn, is the union of the absolute continuous spectrum σ_{ac}, the singular continuous spectrum

σ_{sc}, the eigenvalues of infinite multiplicity, and the limit points of σ_p, where the point spectrum σ_p is the set of eigenvalues (Reed-Simon 1980, p.231,236).

This section concerns the essential spectrum of the Jansen-Hess operator b_m, both for $m = 0$ and $m \neq 0$. In particular, the absence of singular continuous spectrum and embedded eigenvalues will be shown. The strategy of proof is in many cases the same as applied for the corresponding theorems concerning the Brown-Ravenhall operator (EPS 1996, Balinsky and Evans 1998). In these cases, the proofs will only be outlined.

Let us start by recalling the known results for the Brown-Ravenhall operator.

Lemma I.12 (Spectrum of Brown-Ravenhall operator).
Let $b_m^{(1)} = b_{0m} + b_{1m}$, *and assume* $\gamma < \gamma_{BR} = 2/(\frac{\pi}{2} + \frac{2}{\pi})$. *Then*

$$\sigma_{ess}(b_m^{(1)}) \;=\; [m, \infty)$$

$$\sigma_{sc}(b_m^{(1)}) \;=\; \emptyset.$$

$$\text{If } m = 0 \text{ and } \gamma \leq \gamma_{BR}, \qquad \sigma_p(b^{(1)}) \;=\; \emptyset,$$

i.e. $b_m^{(1)}$ *has no singular continuous spectrum and* $b^{(1)} = b_0 + b_1$ *has no eigenvalues, such that* $\sigma(b^{(1)})$ *is absolutely continuous.*

The absence of embedded eigenvalues in the essential spectrum for $m \neq 0$ can be shown with the help of the virial theorem.

Lemma I.13 (Absence of embedded eigenvalues for Brown-Ravenhall operator).
Let $\gamma \leq \gamma_0$. *Then* $b_m^{(1)}$ *has no eigenvalues in* $[m, \infty)$.

This lemma was proven by Balinsky and Evans (1998) for $\gamma_0 = \frac{3}{4}$. By improving their estimates we have obtained $\gamma_0 = \gamma_{BR}$, the maximum possible potential strength for stability of $b_m^{(1)}$. The proof of this new result will be given after the proof of Theorem I.4.

Let us now turn to the Jansen-Hess operator and state our corresponding results.

Theorem I.3.
Let $b_m = b_{0m} + b_{1m} + b_{2m}$ *be the Jansen-Hess operator and assume* $\gamma < \gamma_J$ *with the critical potential strength* $\gamma_J = 1.006$ *as in Lemma I.9. Then*

(i) $\sigma_{ess}(b_m) \;=\; \sigma_{ess}(b_{0m}) \;=\; [m, \infty)$

(ii) $\sigma_{sc}(b_m) \;=\; \emptyset.$

(iii) *If* $m = 0$, $\sigma_p(b) = \emptyset$, *i.e. the spectrum of* b *is absolutely continuous.*

For the proof, one needs the behaviour of b_m under complex dilations. For $\theta := e^{\xi} \in \mathbb{R}_+$, the unitary group of dilation operators d_θ is introduced by means of

$$d_\theta\, \hat{u}(\mathbf{p}) \;=\; \theta^{-3/2}\, \hat{u}(\mathbf{p}/\theta) \;=:\; \hat{u}_\theta(\mathbf{p}) \tag{I.5.1}$$

with $u \in L_2(\mathbb{R}^3) \times \mathbb{C}^2$. Then for $|\xi| < \xi_0$ with a suitably chosen $\xi_0 > 0$, θ is extended to the complex domain $D_{\xi_0} := \{\theta = e^{\xi} :\; \xi \in \mathbb{C},\; |\xi| < \xi_0\}$. One defines the dilated operators

$$b_{m,\theta} :=\; d_\theta\; b_m\; d_\theta^{-1} \tag{I.5.2}$$

and correspondingly $b_{km,\theta} = d_\theta b_{km} d_\theta^{-1}$ for $k = 0, 1, 2$.

When $\theta \in \mathbb{R}_+$, expectation values are invariant under d_θ, such that for $u \in H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2$,

$$(u, b_m\, u) \;=\; (d_\theta\, u, (d_\theta\, b_m\, d_\theta^{-1})\, d_\theta\, u). \tag{I.5.3}$$

In order to derive the explicit form of $b_{m,\theta}$ we make in (I.3.22) the substitution $\mathbf{q} := \theta\mathbf{p}$, $\mathbf{q}' := \theta\mathbf{p}'$ such that

$$(u, b_m\, u) \;=\; \int d\mathbf{q}\, \theta^{-3/2}\, \overline{\hat{u}(\mathbf{q}/\theta)}\, b_{0m}(q/\theta)\, \theta^{-3/2}\, \hat{u}(\mathbf{q}/\theta) \tag{I.5.4}$$

$$+ \int d\mathbf{q}\, \theta^{-\frac{3}{2}}\, \overline{\hat{u}(\mathbf{q}/\theta)} \int d\mathbf{q}'\, \theta^{-3}\, [b_{1m}(\mathbf{q}/\theta, \mathbf{q}'/\theta) \,+ b_{2m}(\mathbf{q}/\theta, \mathbf{q}'/\theta)]\, \theta^{-\frac{3}{2}}\, \hat{u}(\mathbf{q}'/\theta).$$

Upon identification with (I.5.3) one obtains

$$b_{0m,\theta}(p) \;=\; b_{0m}(p/\theta) \;=\; \sqrt{p^2/\theta^2 \,+ m^2} \;=\; \frac{1}{\theta}\, E_p(m\cdot\theta) \;=\; \frac{1}{\theta}\, b_{0m\cdot\theta}(p) \qquad \text{(I.5.5)}$$

$$b_{km,\theta}(\mathbf{p},\mathbf{p}') \;=\; \theta^{-3}\, b_{km}(\mathbf{p}/\theta, \mathbf{p}'/\theta) \;=\; \frac{1}{\theta}\, b_{km\cdot\theta}(\mathbf{p},\mathbf{p}'), \qquad k = 1, 2,$$

where the last equality results from inspection of the explicit expressions (I.3.23) for the kernels of b_{1m} and b_{2m}.

The definition (I.5.5) of the dilated operators $b_{km,\theta}$ in terms of $b_{km\cdot\theta}$ is readily extended to complex $\theta \in D_{\xi_0}$. In the massless case, (I.5.5) reduces to the simple scaling

$$b_{0,\theta}(p) \;=\; \frac{1}{\theta}\, b_0(p), \qquad b_{k,\theta}(\mathbf{p},\mathbf{p}') \;=\; \frac{1}{\theta}\, b_k(\mathbf{p},\mathbf{p}'), \qquad k = 1, 2. \qquad \text{(I.5.6)}$$

Proof outline of (i).
From Lemma I.12 we know that the essential spectrum of $b_{0m} + b_{1m}$ coincides with that of b_{0m}, so it remains to show that adding b_{2m} leads to no changes.

It is known that a compact operator does not change the essential spectrum, however b_{2m} is not bounded from above and hence is not compact. Therefore, the strategy of Weyl's essential spectral theorem (Reed-Simon 1978, p.122) is used: From the compactness of the resolvent difference

$$R_m(\mu) := \;(b_m + \mu)^{-1} \;-\; (b_{0m} + \mu)^{-1} \qquad \text{(I.5.7)}$$

with $\mu \geq 1$ a constant such that the resolvents are bounded (note that $b_{0m} \geq 0$, and b_m is also bounded from below for $\gamma \leq \gamma_J$ according to Lemma I.10), it follows that the essential spectra of b_m and b_{0m} coincide.

With the help of the second resolvent identity, $A^{-1} = B^{-1} - B^{-1}(A - B)A^{-1}$, $R_m(\mu)$ is decomposed,

$$R_m(\mu) \;=\; -(b_{0m} + \mu)^{-1}\, (b_{1m} + b_{2m})\, (b_m + \mu)^{-1} \qquad \text{(I.5.8)}$$

$$= \;-\left\{(b_{0m} + \mu)^{-1}\, (b_{1m} + b_{2m})\, (b_{0m} + \mu)^{-1/2}\right\}\; \left[(b_{0m} + \mu)^{1/2}\, (b_m + \mu)^{-1}\right]$$

and it is shown that $R_m(\mu)$ is compact by means of compactness of the term in curly brackets and boundedness of the second factor.

To show boundedness of the term in square brackets we split off the bounded operator $(b_m + \mu)^{-1/2}$. Boundedness of $(b_{0m} + \mu)^{1/2}(b_m + \mu)^{-1/2}$ results from the b_{0m}-form boundedness of b_m (Proposition I.4) expressed as

$$(\psi,\, (b_{1m} + b_{2m})\, \psi) \;\geq\; -(1 - \epsilon)\, (\psi, b_{0m}\, \psi) \;-\; C\, (\psi, \psi). \qquad \text{(I.5.9)}$$

From this we obtain with $\psi := (b_m + \mu)^{-1/2}\, u$ the required boundedness condition

$$\|(b_{0m}{+}\mu)^{1/2}\, (b_m{+}\mu)^{-1/2}\, u\|^2 \;=\; (\psi,\, (b_{0m}{+}\mu)\, \psi) \;\leq\; c_0\, \|u\|^2 \;=\; c_0\, (\psi,\, (b_m{+}\mu)\, \psi) \qquad \text{(I.5.10)}$$

upon the choices $c_0 \geq 1/\epsilon$ and $\mu > \max\{1, c_0 C/(c_0 - 1)\}$.

Compactness concerning the first-order contribution, b_{1m}, to the factor in curly brackets, was shown by EPS (1996). Their proof is based on Lemma 2.6 of Herbst (1977) which states that the operator $(b_{0m} + \mu)^{-1}\, \frac{1}{\sqrt{x}}$ is compact. For the second-order contribution, b_{2m}, we use the Sobolev representation (I.3.24) and (I.3.30) of operators and introduce the following factorisation

$$(D_0 \,+\, \mu)^{-1}\, B_{2m}\, (D_0 \,+\, \mu)^{-1/2} \;=\; \frac{\gamma^2}{8\pi^2}\, \left\{(D_0 + \mu)^{-1} \frac{1}{\sqrt{x}}\right\} \qquad \text{(I.5.11)}$$

$$\cdot \left[\frac{1}{\sqrt{x}} \, (1 - \tilde{D}_0(\mathbf{p}))(E_p + \mu)^{-1/2} \right] \, \left[(E_p + \mu)^{1/2} \, V_{10,m} \, (D_0 + \mu)^{-1/2} \right]$$

$$+ \frac{\gamma^2}{8\pi^2} \left[(D_0 + \mu)^{-1} V_{10,m} (1 - \tilde{D}_0(\mathbf{p}))(E_p + \mu) \right] \left\{ (E_p + \mu)^{-1} \frac{1}{\sqrt{x}} \right\} \left[\frac{1}{\sqrt{x}} \, (D_0 + \mu)^{-1/2} \right].$$

Since these operators act on the positive spectral subspace of D_0, the lemma of Herbst (1977) assures that the operators in curly brackets in (I.5.11) are compact. The operators in square brackets are readily shown to be bounded by using that $\tilde{D}_0(\mathbf{p})$ is bounded as is $V_{10,m}$ (see (I.4.22)), and by applying Kato's (1966) inequality, $1/x \leq \frac{\pi}{2}\, p$, to the terms involving $\frac{1}{\sqrt{x}}\,(D_0 + \mu)^{-1/2}$. For example, using the Lieb and Yau formula (Lemma I.1), one can estimate for $\varphi \in \mathcal{H}_{+,1}$

$$\|(E_p + \mu)^{1/2} \; V_{10,m} \; (D_0 + \mu)^{-1/2} \; \varphi\|^2 \qquad \text{(I.5.12)}$$

$$= \int d\mathbf{p} \left| (E_p + \mu)^{1/2} \int d\mathbf{p}' \; \frac{1}{|\mathbf{p} - \mathbf{p}'|^2} \; \frac{1}{E_p + E_{p'}} \; (E_{p'} + \mu)^{-1/2} \; \hat{\varphi}(\mathbf{p}') \right|^2$$

$$\leq \int d\mathbf{p}' \; |\hat{\varphi}(\mathbf{p}')|^2 \cdot \int d\mathbf{p} \; |K(\mathbf{p}', \mathbf{p})| \; \frac{f(p')}{f(p)}$$

with $K(\mathbf{p}', \mathbf{p}) := \int d\mathbf{q} \, k((\mathbf{q}, \mathbf{p}') \, k(\mathbf{q}, \mathbf{p})$ and

$$k(\mathbf{q}, \mathbf{p}) := \; (E_q + \mu)^{1/2} \; \frac{1}{|\mathbf{q} - \mathbf{p}|^2} \; \frac{1}{E_q + E_p} \; (E_p + \mu)^{-1/2}. \qquad \text{(I.5.13)}$$

Choosing $f(p) = p^{3/2}$ and estimating $(E_q + E_p)^{-1}$ by $(q + m)^{-1}$ for $m \neq 0$ (while substituting $\mathbf{p} =: q\mathbf{p}''$ for $m = 0$) in the integral over $\mathbf{p}$, it is straightforward to verify that the integral over the kernel in (I.5.12) is finite. (For a more detailed proof within the Douglas-Kroll representation of operators, see JA (2002).) ■

Proof outline of (ii).

Concerning the absence of the singular continuous spectrum, one has to show that the family of bounded operators $(b_{0m} + \mu)^{-1/2}(b_{1m,\theta} + b_{2m,\theta})(b_{0m} + \mu)^{-1/2}$ extends to an analytic operator-valued function in D_{ξ_0} (EPS 1996, JA 2002). The dilated functions $d_\theta u$ are also analytic in D_{ξ_0}, provided $u \in \mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^2$ which is a dense subspace of $H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2$ (Folland 1995, p.192).

For $\theta \in \mathbb{R} \cap D_{\xi_0}$ and $z \in \mathbb{C} \backslash \mathbb{R}$, one has invariance of the (finite) resolvent expectation value under dilations,

$$(u, \; \frac{1}{b_m - z} \, u) \; = \; (d_\theta \, u, \; \frac{1}{b_{m,\theta} - z} \, d_\theta \, u). \qquad \text{(I.5.14)}$$

However, because of the identity theorem from complex analysis, analyticity of $d_\theta u$ and of $b_{m,\theta}$ guarantees (I.5.14) for all $\theta \in D_{\xi_0}$. Moreover, since $\mathcal{S}$ is dense in $H_{1/2}$, (I.5.14) holds for all $u \in H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2$.

The essential spectrum of $b_{m,\theta}$ is the same as that of $b_{0m,\theta}$, which again is shown by proving the compactness of the resolvent difference $R_{m,\theta}(\mu) := (b_{m,\theta} + \mu)^{-1} - (b_{0m,\theta} + \mu)^{-1}$, along the lines indicated in the proof of (i).

We note that for fixed $\theta = \exp(x + iy)$, $\sigma_{ess}(b_{0m,\theta}) = \{b_{0m,\theta}(p) : p \in [0, \infty)\} = \{\sqrt{p^2/\theta^2 + m^2} \; : \; p \in [0, \infty)\}$. Hence for $m = 0$ it is the nonnegative real axis rotated by the angle $-y$ around the origin, and for $m \neq 0$ it is a curve in the complex plane intersecting $\mathbb{R}$ only at the point m.

Therefore, apart from isolated points, the resolvent sets of $b_{0m,\theta}$ and $b_{m,\theta}$ (which are the complementary sets of the spectrum σ in $\mathbb{C}$) agree and coincide due to (I.5.14) also with the resolvent set of b_m. Since there exists only one intersection point of $\sigma_{ess}(b_{m,\theta})$ with $\mathbb{R}_+$, we have

$$\lim_{\text{Im}z \to 0} \; \text{Im} \; (u, \frac{1}{b_m - z} \, u) \; < \; \infty \qquad \text{(I.5.15)}$$

except at isolated points of $\mathbb{R}_+$. From this it follows that the singular continuous spectrum is absent (Reed-Simon 1978, §XIII.6, XIII.10; EPS 1996). ■

Proof of (iii).
We have to show that for $m = 0$, b has no eigenvalues.

First assume $E \neq 0$ is an eigenvalue of b, i.e. there exists $u \in H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2$ such that $b\,u = Eu$. Due to the scaling property (I.5.6), we have for $\theta \in D_{\xi_0} \cap \mathbb{R}_+$

$$(d_\theta\, b\, d_\theta^{-1})\; u_\theta \;=\; \frac{1}{\theta}\, b\, u_\theta \;=\; E\, u_\theta \tag{I.5.16}$$

such that θE is eigenvalue of b. Since, however, $D_{\xi_0} \cap \mathbb{R}_+$ is overcountable, there is an overcountable basis of eigenvectors u_θ which contradicts the separability of the Hilbert space $H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2$.

Assume now $E = 0$ is an eigenvalue of b, i.e. there exists $u \neq 0$ such that $b\,u = 0$. Using the partial wave decomposition introduced in Appendix B, we have from (B.7) in Mellin space

$$0 \;=\; (u, b\,u) \;=\; \sum_\nu \int_{-\infty}^{\infty} dt\; |a_\nu^\#(t + i/2)|^2\; b_{ls}^\#(t - i/2) \tag{I.5.17}$$

where $b_{ls}^\#(t - \frac{i}{2}) \;=\; 1 + \sqrt{2\pi}(\; b_{ls}^{(1)\#} \;+\; b_{ls}^{(2)\#})(t - \frac{i}{2})$. However, positivity of b for $\gamma < \gamma_J$ results from $b_{ls}^\#(t - \frac{i}{2})$ being strictly positive. Therefore, the r.h.s. of (I.5.17) can only be zero if for each ν,

$$|a_\nu^\#(t + i/2)| \;=\; 0 \qquad \text{almost everywhere for } t \in \mathbb{R}. \tag{I.5.18}$$

If $u \in \mathcal{S}(\mathbb{R}^3) \times \mathbb{C}^2$ then $a_\nu^\#$ is an analytic function in the strip $\{\tau = t + is \in \mathbb{C} : -\infty < t < \infty,\; 0 \le s \le \frac{1}{2}\}$. From the identity theorem it follows that $a_\nu^\#(t) = 0$ for all $t \in \mathbb{R}$. Unitarity of the Mellin transform gives

$$0 \;=\; \sum_\nu \int_{-\infty}^{\infty} dt\; |a_\nu^\#(t)|^2 \;=\; \sum_\nu \int_0^{\infty} dp\; |a_\nu(p)|^2 \;=\; \|u\|^2, \tag{I.5.19}$$

hence $u = 0$. Since $\mathcal{S}$ is dense in $H_{1/2}$ we have $u = 0$ in $H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2$, a contradiction. ■

Our last result is a generalisation of Lemma I.13 to the massive Jansen-Hess operator.

Theorem I.4.
Let b_m be the massive Jansen-Hess operator and assume $\gamma < \gamma_J = 1.006$. Then the eigenvalues λ of b_m are confined to $\lambda \le m(1 + s(\gamma))$ with

$$s(\gamma) := \max\{0,\, s_0(m_1\gamma - m_0 + m_2\gamma^2)\} \tag{I.5.20}$$

where $s_0 := 5$, $m_0 := 0.3058$, $m_1 := \frac{2}{5}$ and $m_2 := 2.253$. In particular, for $\gamma < 0.29$ ($Z < 40$) the essential spectrum of b_m has no embedded eigenvalues.

Proof. For an operator b_m with the scaling property (I.5.5) under dilations d_θ, Balinsky and Evans (1998; Lemma 2.1) formulated the following virial theorem

$$\lim_{\theta \to 1} (u_\theta,\, \frac{b_{m\cdot\theta} - b_m}{\theta - 1}\, u) \;=\; \lambda\, \|u\|^2 \tag{I.5.21}$$

for $\theta \in \mathbb{R}_+$. In order to interchange the limit $\theta \to 1$ with the spatial integration, the uniform absolute convergence of the form on the l.h.s. of (I.5.21) is needed.

In order to show this, we rely on the proofs of form boundedness of $\left|\dfrac{db_{km}}{dm}\right|$, $k = 1, 2,$ by Stockmeyer (2002) for $k = 1$ and BSS (2002) for $k = 2$, when establishing Lemma I.8(ii) and Lemma I.10(i). In the present case, we only have to replace

$m \mapsto m \cdot \theta \in \mathbb{R}_+$ and use the Lieb and Yau formula for off-diagonal forms (Lemma I.2).

Defining $m_1 := \min\{m, m\cdot\theta\}$ and $M_1 := \max\{m, m\cdot\theta\}$, and applying the mean value theorem with $\xi \in (m_1, M_1)$, we thus obtain with $\|u_\theta\| = \|u\|$,

$$\left|(u_\theta, \frac{b_{m\cdot\theta} - b_m}{\theta - 1}\, u)\right| \le (|u_\theta|, m \left|\frac{db_{m\cdot\theta}}{dm\cdot\theta}(\xi)\right| |u|) \le mc\,\|u\|^2 \tag{I.5.22}$$

with some constant c, such that the dominated convergence theorem applies. Thus, carrying out the limit in (I.5.21) we get

$$\lambda\,\|u\|^2 = m^2 \int d\mathbf{p}\, |\hat{u}(\mathbf{p})|^2\, \frac{1}{E_p}$$
$$+\, m \int d\mathbf{p} d\mathbf{p}'\, \overline{\hat{u}(\mathbf{p})} \left(\frac{db_{1m}(\mathbf{p},\mathbf{p}')}{dm} + \frac{db_{2m}(\mathbf{p},\mathbf{p}')}{dm}\right) \hat{u}(\mathbf{p}'). \tag{I.5.23}$$

Therefore upon differentiating (I.3.23) the term linear in the coupling constant can be written in the following way

$$\int d\mathbf{p}\, d\mathbf{p}'\, \overline{\hat{u}(\mathbf{p})}\, \frac{db_{1m}(\mathbf{p},\mathbf{p}')}{dm}\, \hat{u}(\mathbf{p}')$$
$$= \operatorname{Re} \int d\mathbf{p}\, d\mathbf{p}'\, \overline{\hat{u}(\mathbf{p})} \left(\frac{1}{E_p} - \frac{m}{E_p^2}\right) b_{1m}(\mathbf{p},\mathbf{p}')\, \hat{u}(\mathbf{p}')$$
$$+\frac{\gamma}{2\pi^2} \int d\mathbf{p}\, d\mathbf{p}'\, \overline{\hat{u}(\mathbf{p})}\, \frac{1}{|\mathbf{p}-\mathbf{p}'|^2} A(p)A(p')\boldsymbol{\sigma}\hat{\mathbf{p}}\boldsymbol{\sigma}\hat{\mathbf{p}}' h(p)\, h(p') \left(\frac{1}{E_p} + \frac{1}{E_p'}\right) \hat{u}(\mathbf{p}'). \tag{I.5.24}$$

The first term in (I.5.24) carrying the negative sign of b_{1m} is eliminated with the help of the eigenvalue equation in the form

$$(\psi, b_m\, u) = \int d\mathbf{p}\, \overline{\psi(\mathbf{p})} E_p \hat{u}(\mathbf{p}) + \int d\mathbf{p}\, d\mathbf{p}'\, \overline{\psi(\mathbf{p})}\, [b_{1m}(\mathbf{p},\mathbf{p}') + b_{2m}(\mathbf{p},\mathbf{p}')]\, \hat{u}(\mathbf{p}')$$
$$= (\psi, \lambda\, u)$$
$$\psi(\mathbf{p}) := \left(\frac{1}{E_p} - \frac{m}{E_p^2}\right) \hat{u}(\mathbf{p}). \tag{I.5.25}$$

This procedure of eliminating a negative first-order term at the expense of additional zero-order terms (for which no further estimate is needed) and second-order terms (which are small for small γ) is mandatory for the desired estimate on the eigenvalue λ. With (I.5.24) and (I.5.25), the virial theorem (I.5.23) results in

$$\frac{\lambda}{m}\,\|u\|^2 = \int d\mathbf{p}\, |\hat{u}(\mathbf{p})|^2 \left(\frac{m}{E_p} + (\frac{\lambda}{E_p} - 1)(1 - \frac{m}{E_p})\right) + \frac{\gamma}{2\pi^2} \int d\mathbf{p}\, d\mathbf{p}'\, \overline{\hat{u}(\mathbf{p})}$$
$$\cdot A(p)\, A(p') \left[\frac{1}{|\mathbf{p}-\mathbf{p}'|^2} \boldsymbol{\sigma}\hat{\mathbf{p}}\, \boldsymbol{\sigma}\hat{\mathbf{p}}' h(p)\, h(p') \left(\frac{1}{E_p} + \frac{1}{E_{p'}}\right) + \frac{\gamma}{4\pi^2}\, T_2(\mathbf{p},\mathbf{p}')\right] \hat{u}(\mathbf{p}') \tag{I.5.26}$$

where the lengthy expression for $T_2(\mathbf{p},\mathbf{p}')$, originating from the derivative of the second-order term $b_{2m}(\mathbf{p},\mathbf{p}')$, is given in Appendix H.

Applying the Lieb and Yau formula, Lemma I.1, with $\hat{\psi}(\mathbf{p}) \mapsto A(p)h(p)\, \hat{u}(\mathbf{p})$ and $A(p)\, \hat{u}(\mathbf{p})$, respectively, to the first-order and second-order term, and estimating $|\boldsymbol{\sigma}\hat{\mathbf{p}}\, \boldsymbol{\sigma}\hat{\mathbf{p}}'|$ by unity, one obtains

$$\left(\frac{\lambda}{m} - 1\right) \int d\mathbf{p}\, |\hat{u}(\mathbf{p})|^2 \left(1 - \frac{m}{E_p} + \frac{m^2}{E_p^2}\right) \le -\int d\mathbf{p}\, |\hat{u}(\mathbf{p})|^2 \frac{(E_p - m)(2E_p - m)}{E_p^2}$$
$$+\, \frac{\gamma}{2\pi^2} \int d\mathbf{p}\, |\hat{u}(\mathbf{p})|^2\, A(p)^2 \left\{ h^2(p) \int d\mathbf{p}'\, \frac{1}{|\mathbf{p}-\mathbf{p}'|^2} \left(\frac{1}{E_p} + \frac{1}{E_{p'}}\right) \frac{f(p)}{f(p')}\right.$$

$$+ \ \frac{\gamma}{4\pi^2} \int d\mathbf{p}' \ |T_2(\mathbf{p},\mathbf{p}')| \ \frac{f(p)}{f(p')} \Big\} \tag{I.5.27}$$

The last term in (I.5.27) can be further estimated by breaking $T_2(\mathbf{p},\mathbf{p}')$ from (H.1) into its constituents and estimating each contribution separately as indicated in Appendix H. Recalling that the convergence generating functions can be chosen differently for each integral, functions of the type $f(p) = p^{3/2}$ as well as $f(p) = p^{3/2} \, \frac{p}{e(p)}$ with $e(p) \in \{E_p, E_p + m, p + m\}$ are selected in order to optimise the estimates. Further, the following estimate is used in the evaluation of the integrals over p',

$$\frac{1}{\sqrt{(qp')^2+1}\,+c} \ \le \ \begin{cases} \dfrac{1}{1+c}, & p' \le 1/q \\[2ex] \dfrac{1}{qp'}, & p' > 1/q \end{cases} , \qquad c \ge 0, \ q \ge 0\,. \tag{I.5.28}$$

Defining $\mathbf{q} := \mathbf{p}/m$, denoting the estimate of $\int d\mathbf{p}' \, |T_2(\mathbf{p},\mathbf{p}')| \, f(p)/f(p')$ by $(4\pi^2)^2 q^2 M_2(q)$, and taking $f(p) := p^{3/2}$ in the term linear in γ, such that with formula (A.1), the substitution $q' := p'/mq$ for p' and (I.5.28),

$$\int d\mathbf{p}' \, \frac{1}{|\mathbf{p}-\mathbf{p}'|^2} \, \frac{1}{E_p'} \left(\frac{p}{p'}\right)^{3/2} \ \le \ 4\pi^2 \, \alpha(q) \tag{I.5.29}$$

$$\alpha(q) := 1 + \frac{1}{\pi}\left(2\sqrt{q}\,\ln\left|\frac{1+q}{1-q}\right| + 2\,(q-1)\,\arctan\frac{1}{\sqrt{q}} - (q+1)\,\ln\left|\frac{1+\sqrt{q}}{1-\sqrt{q}}\right|\right),$$

we arrive at the following estimate

$$0 \ \le \ m^3 \int d\mathbf{q} \, |\hat{u}(m\mathbf{q})|^2 \left(1 - \frac{1}{\sqrt{q^2+1}} + \frac{1}{q^2+1}\right) \left(1 - \frac{\lambda}{m} + \phi(q)\right) \tag{I.5.30}$$

$$\phi(q) := \frac{q^2}{q^2+2-\sqrt{q^2+1}} \, \frac{1}{f_0(q)} \, \left(-g_0(q) \ + \ \gamma g_1(q) \ + \ \gamma^2 g_2(q)\right) \, f_0(q)$$

where

$$g_0(q) := \frac{2\sqrt{q^2+1}-1}{\sqrt{q^2+1}+1}, \qquad g_1(q) := \frac{q+\alpha(q)\sqrt{q^2+1}}{\sqrt{q^2+1}+1}$$

$$g_2(q) := \ (q^2+1+\sqrt{q^2+1})\,M_2(q), \qquad f_0(q) := \frac{q+c}{aq+b} \tag{I.5.31}$$

are nonnegative bounded functions. The auxiliary function f_0 with $a, b, c > 0$ has been introduced to improve on the estimate of ϕ. It follows from (I.5.30) that for $\phi < 0$, $\lambda < m$ since the factor multiplying the last bracket is nonnegative. With $m_0 := \inf g_0 f_0$, $m_1 := \sup g_1 f_0$ and $m_2 := \sup g_2 f_0$ for $0 \le q < \infty$, this condition on ϕ is fulfilled for $-m_0 + m_1\gamma + m_2\gamma^2 < 0$, i.e. $\gamma < \gamma_0$, say. For $a := 5$, $b := \frac{1}{5}$, $c := 1.1$, we obtain $m_0 = 0.3058$, $m_1 = \frac{2}{5}$, $m_2 = 2.253$, and hence $\gamma_0 = 0.29$. This improves on the value $\gamma_0 = 0.159$ obtained for $f_0 = 1$ (where $m_0 = \frac{1}{2}$, $\sup g_1 = 2$, $\sup g_2 = \frac{29}{4}$). Denoting by s_0 the supremum of the prefactor of $\phi(q)$ in $q \in \mathbb{R}^+$, $s_0 := \sup q^2/(q^2+2-\sqrt{q^2+1})\, f_0^{-1}(q) = 5$, we can estimate $\phi(q)$ for $\gamma > \gamma_0$ to obtain from (I.5.30)

$$\lambda \ \le \ m\,(1 + \phi(q)) \ \le \ m\,(1 \ + \ s_0(m_1\gamma - m_0 + m_2\gamma^2)), \tag{I.5.32}$$

which proves the theorem. ∎

In the Brown-Ravenhall case, Lemma I.13, we have derived the improved critical potential strength γ_0 by setting $g_2 \equiv 0$ in $\phi(q)$. Thus we have the estimate (I.5.30) with λ replaced by $\tilde{\lambda}$, the eigenvalue of $b_m^{(1)}$, and with $\phi(q)$ now defined by

$$\phi(q) := \frac{q^2}{q^2 + 2 - \sqrt{q^2+1}}\, g_1(q) \left(\gamma - \frac{g_0(q)}{g_1(q)} \right). \tag{I.5.33}$$

We obtain $\phi(q) < 0$ for $\gamma < \min\limits_{q \in \mathbb{R}_+} \frac{g_0(q)}{g_1(q)} = 0.973 =: \tilde{\gamma}_0$. In particular, $\phi(q) < 0$ and hence $\tilde{\lambda} < m$ for $\gamma \leq \gamma_{BR} = 0.906$.

Note that Balinsky and Evans (1998) did not use the improved estimate (I.5.28) for small p', but rather $1/qp'$ throughout. This results in $\alpha(q) = 1$ in place of (I.5.29).

II. Two-Electron Ions

The generalisation of the one-electron Dirac theory to an N-electron atom leads to the Coulomb-Dirac operator (Sucher 1958, Douglas and Kroll 1974)

$$H \;=\; \sum_{k=1}^{N} (D_0^{(k)} + V^{(k)}) \;+\; P_{+,N} \sum_{n<k}^{N} \frac{e^2}{|\mathbf{x}_n - \mathbf{x}_k|} \, P_{+,N} \tag{II.1}$$

in the Hilbert space $\mathcal{A}\,(L_2(\mathbb{R}^3) \times \mathbb{C}^4)^N$ where $\mathcal{A}$ denotes antisymmetrisation of the N-electron wavefunction with respect to the interchange of any two electrons. The form domain of H is the subspace $\mathcal{H}_N := \mathcal{A}(H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4)^N$. Here, $D_0^{(k)} = \boldsymbol{\alpha}^{(k)}\mathbf{p}^{(k)} + \beta^{(k)} m$ is the free Dirac operator of electron k, $V^{(k)}$ its central Coulomb potential, and the second sum runs over all values of n and k from 1 to N with the restriction $n < k$. The projector $P_{+,N} = \bigotimes_{k=1}^{N} P_+^{(k)}$ is a direct product of the single-particle projectors $P_+^{(k)}$ onto the positive spectral subspace of $H^{(k)} = D_0^{(k)} + V^{(k)}$.

II.1. **The independent-particle model.**

Let us assume that H can be approximated by a sum of identical one-particle operators $h^{(k)}$, which are obtained from a self-consistent field (Hartree-Fock) approach (Landau and Lifschitz 1965, §69; Sucher 1980),

$$H \;=\; \sum_{k=1}^{N} h^{(k)}. \tag{II.1.1}$$

For noninteracting particles, $\psi \in \mathcal{H}_N$ can be chosen as Slater determinant composed of the single-particle states $\varphi_1, ..., \varphi_N$. Then one gets

$$(\psi, H\psi) \;=\; \sum_{k=1}^{N} (\varphi_k, h^{(k)}\, \varphi_k), \tag{II.1.2}$$

which is just a superposition of the one-particle expectation values. One should keep in mind, however, the restriction on the set $(\varphi_k)_{k=1,\ldots,N}$ to provide a non-vanishing Slater determinant.

In this case, the Sobolev transformation scheme applied to H leads to a simple result. Since operators acting on distinct particles commute, the transformed operator to order n is represented as a sum over (identical) one-particle contributions, compare (I.2.11) and (I.2.12),

$$H^{(n)} \;=\; \sum_{k=1}^{N} \left(D_0^{(k)} \,+\, \tilde{V}_1^{(k)} \,+\, ... +\, \tilde{V}_n^{(k)} \right) \tag{II.1.3}$$

where in the definition of the i-th order potential terms $\tilde{V}_i^{(k)}$ $(i = 1, 2, ..., n)$, the Coulomb field $V^{(k)} = -\gamma/x_k$ is everywhere replaced by the effective Hartree-Fock single-particle potential contained in $h^{(k)}$. In general, this effective potential consists of Coulomb-type and bounded contributions. Hence, the single-particle results of part I concerning relative form boundedness and positivity hold also in the case of independent particles.

II.2. **Unitary transformations.**

Let us abandon the independent-particle model and include the electron-electron correlations inherent in the Coulomb-Dirac operator (II.1). In the following we will only consider the two-electron case ($N = 2$). Let $\psi \in \mathcal{H}_{+,2} := (\Lambda_+^{(1)} \otimes \Lambda_+^{(2)})(\mathcal{A}(H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4)^2)$ be an antisymmetrised two-particle spinor in the positive spectral subspace of the free Dirac operator, that means

$$\Lambda_+^{(1)}\Lambda_+^{(2)}\,\psi \;=\; \psi, \quad \Lambda_+^{(1)}\Lambda_-^{(2)}\,\psi \;=\; \Lambda_-^{(1)}\Lambda_+^{(2)}\,\psi \;=\; \Lambda_-^{(1)}\Lambda_-^{(2)}\,\psi \;=\; 0 \tag{II.2.1}$$

where for brevity we write $\Lambda^{(1)}\Lambda^{(2)}$ for $\Lambda^{(1)} \otimes \Lambda^{(2)}$. Our aim is to apply the Sobolev transformation scheme to the two-particle operator (II.1), such that the transformed Coulomb-Dirac operator takes the block-diagonal form $U^+ H U = H^{(n)} + R((e^2)^{n+1})$ with

$$H^{(n)} := \;\mathrm{proj}\,(A) := \;\Lambda_+^{(1)}\Lambda_+^{(2)}\,A\,\Lambda_+^{(1)}\Lambda_+^{(2)} + \Lambda_-^{(1)}\Lambda_-^{(2)}\,A\,\Lambda_-^{(1)}\Lambda_-^{(2)} + \Lambda_+^{(1)}\Lambda_-^{(2)}\,A\,\Lambda_+^{(1)}\Lambda_-^{(2)}$$

$$+\,\Lambda_-^{(1)}\Lambda_+^{(2)}\,A\,\Lambda_-^{(1)}\Lambda_+^{(2)}, \tag{II.2.2}$$

where A is an operator to be determined later, and R is the remainder which is of order $(e^2)^{n+1}$. In contrast to the one-particle case, the expansion parameter is the fine structure constant e^2, rather than the strength $\gamma = Ze^2$ of the central potential. The operator A in (II.2.2) includes terms to order n in e^2.

We start by using the integral representation of the projectors $P_+^{(k)}$, $\Lambda_+^{(k)}$ (Kato 1966, Chap.II, §1.3)

$$P_+^{(k)} \;=\; \frac{1}{2} + \frac{1}{2\pi}\int_{-\infty}^{\infty} d\eta\,\frac{1}{D_0^{(k)} + V^{(k)} + i\eta}, \qquad \Lambda_+^{(k)} \;=\; \frac{1}{2} + \frac{1}{2\pi}\int_{-\infty}^{\infty} d\eta\,\frac{1}{D_0^{(k)} + i\eta} \tag{II.2.3}$$

to express $P_+^{(k)}$ in terms of the free projector $\Lambda_+^{(k)}$ with the help of the resolvent identity,

$$\frac{1}{D_0^{(k)} + V^{(k)} + i\eta} \;=\; \frac{1}{D_0^{(k)} + i\eta} \;-\; \frac{1}{D_0^{(k)} + i\eta}\,V^{(k)}\,\frac{1}{D_0^{(k)} + V^{(k)} + i\eta}, \tag{II.2.4}$$

giving

$$P_+^{(k)} \;=\; \Lambda_+^{(k)} \;-\; \frac{1}{2\pi}\int_{-\infty}^{\infty} d\eta\,\frac{1}{D_0^{(k)} + i\eta}\,V^{(k)}\,\frac{1}{D_0^{(k)} + V^{(k)} + i\eta} \tag{II.2.5}$$

$$=:\; \Lambda_+^{(k)} \;+\; F_V^{(k)}.$$

Then the two-particle term of H turns into

$$P_+^{(1)}P_+^{(2)}\,V^{(12)}\,P_+^{(1)}P_+^{(2)} \;=\; \Lambda_+^{(1)}\Lambda_+^{(2)}\,V^{(12)}\,\Lambda_+^{(1)}\Lambda_+^{(2)} \;+\; F_V^{(1)}\Lambda_+^{(2)}\,V^{(12)}\,\Lambda_+^{(1)}\Lambda_+^{(2)}$$

$$+\,F_V^{(2)}\Lambda_+^{(1)}\,V^{(12)}\,\Lambda_+^{(1)}\Lambda_+^{(2)} \;+\; \Lambda_+^{(1)}\Lambda_+^{(2)}\,V^{(12)}\,\Lambda_+^{(2)}F_V^{(1)} \;+\; \Lambda_+^{(1)}\Lambda_+^{(2)}\,V^{(12)}\,\Lambda_+^{(1)}F_V^{(2)} \;+\; R \tag{II.2.6}$$

where $V^{(12)} := \dfrac{e^2}{|\mathbf{x}_1 - \mathbf{x}_2|}$ and R comprises the remaining terms which are of order $(e^2)^3$.

Since the linear term in e^2 (the first term on the r.h.s of (II.2.6)) has already the desired block-diagonal structure of (II.2.2), the first Sobolev transformation

$$U_1 \;=\; e^{iB_1} \;:=\; e^{i(B_1^{(1)} + B_1^{(2)})} \tag{II.2.7}$$

can be restricted to a sum of the one-particle self-adjoint operators $B_1^{(k)}$ from chapter I. Thereby use is made of the fact that all single-particle operators pertaining to particle 1 commute with those of particle 2. One obtains, using the defining equation (I.2.10) for the operators $B_1^{(k)}$,

$$U_1^{-1}\,H\,U_1 \;=\; \sum_{k=1}^{2}\left(D_0^{(k)} \,+\, V_1^{(k)} \,+\, i\,[V_1^{(k)},B_1^{(k)}] \,+\, \frac{i}{2}\,[W_1^{(k)},B_1^{(k)}]\right)$$

$$+\,\Lambda_+^{(1)}\Lambda_+^{(2)}\,V^{(12)}\,\Lambda_+^{(1)}\Lambda_+^{(2)} \;+\; i\,[\Lambda_+^{(1)}\Lambda_+^{(2)}\,V^{(12)}\,\Lambda_+^{(1)}\Lambda_+^{(2)},B_1^{(1)}+B_1^{(2)}] \qquad \text{(II.2.8)}$$

$$+(F_0^{(1)}\Lambda_+^{(2)}+F_0^{(2)}\Lambda_+^{(1)})V^{(12)}\Lambda_+^{(1)}\Lambda_+^{(2)}+\Lambda_+^{(1)}\Lambda_+^{(2)}V^{(12)}(\Lambda_+^{(2)}F_0^{(1)}+\Lambda_+^{(1)}F_0^{(2)})+R((e^2)^3)$$

where

$$F_0^{(k)} \;:=\; -\frac{1}{2\pi}\int_{-\infty}^{\infty}d\eta\;\frac{1}{D_0^{(k)}+i\eta}\;V^{(k)}\;\frac{1}{D_0^{(k)}+i\eta}, \qquad k=1,2 \qquad \text{(II.2.9)}$$

is the first-order term in e^2 of the iteration obtained for $F_V^{(k)}$ by successive insertion of the resolvent identity (II.2.4).

For any operator C we introduce the decomposition by means of $1\cdot C\cdot 1$ with $1=(\Lambda_+^{(1)}+\Lambda_-^{(1)})(\Lambda_+^{(2)}+\Lambda_-^{(2)})$,

$$C \;=\; \text{proj}\;(C) \;+\; \text{off}\;(C), \qquad \text{(II.2.10)}$$

where proj (C) is defined in (II.2.2) and off (C) contains all nondiagonal combinations of the projectors. We identify C with all terms in (II.2.8) which are of second order in e^2, and eliminate off (C) by means of the second Sobolev transformation U_2 in an analogous way as in the one-particle case. Explicitly,

$$U_2 \;=\; e^{iB_2}, \qquad B_2 \;=\; B_2^{(1)} \,+\, B_2^{(2)} \,+\, B_2^{(12)} \qquad \text{(II.2.11)}$$

where $B_2^{(k)}$ are one-particle operators affecting only particle k while $B_2^{(12)}$ is a two-particle operator. B_2 is defined by

$$\text{off}\;(C) \;=\; -i\;[(D_0^{(1)}+D_0^{(2)}),\,B_2^{(1)}\,+B_2^{(2)}\,+B_2^{(12)}]. \qquad \text{(II.2.12)}$$

Accordingly, C is decomposed into single- and two-particle contributions, $C = C^{(1)}+C^{(2)}+C^{(12)}$ with

$$C^{(k)} \,:=\; i\,[V_1^{(k)},B_1^{(k)}] \,+\, \frac{i}{2}\,[W_1^{(k)},B_1^{(k)}], \qquad k=1,2$$

$$C^{(12)} \,:=\; i\,\sum_{k=1}^{2}\,[\Lambda_+^{(1)}\Lambda_+^{(2)}\,V^{(12)}\,\Lambda_+^{(1)}\Lambda_+^{(2)},B_1^{(k)}] \qquad \text{(II.2.13)}$$

$$+\;(F_0^{(1)}\Lambda_+^{(2)}\;+\;F_0^{(2)}\Lambda_+^{(1)})\;V^{(12)}\,\Lambda_+^{(1)}\Lambda_+^{(2)}\;+\;\Lambda_+^{(1)}\Lambda_+^{(2)}\,V^{(12)}\,(\Lambda_+^{(2)}F_0^{(1)}\;+\;\Lambda_+^{(1)}F_0^{(2)}).$$

Since off (C) is linear in C, (II.2.12) is satisfied if we define the single-particle operators as done earlier, using the projector property $(\Lambda_\pm^{(k)})^2=\Lambda_\pm^{(k)}$,

$$\text{off}\,(C^{(k)}) \;=\; \Lambda_+^{(k)}\,C^{(k)}\,\Lambda_-^{(k)} \;+\; \Lambda_-^{(k)}\,C^{(k)}\,\Lambda_+^{(k)} \;=\; -i\,[D_0^{(k)},B_2^{(k)}], \qquad k=1,2 \qquad \text{(II.2.14)}$$

and

$$\text{off}\,(C^{(12)}) \;=:\; W^{(12)} \;=\; -i\,[(D_0^{(1)}+D_0^{(2)},B_2^{(12)}]. \qquad \text{(II.2.15)}$$

We collect our results in the following proposition.

Proposition II.1 (Existence of Sobolev transformations).
Let $U_1=e^{iB_1}$, $U_2=e^{iB_2}$ be the Sobolev transformations such that the transformed two-particle Coulomb-Dirac operator $(U_1U_2)^{-1}\,H\,U_1U_2$ has the block-diagonal projector form of (II.2.2) up to second order in the coupling constant e^2. Then B_1 and B_2 are self-adjoint bounded operators on $(L_2(\mathbb{R}^3)\times\mathbb{C}^4)^2$.

The boundedness of B_2 is shown in the next setion. Then the self-adjointness of $B^{(12)}$ follows immediately from the defining equation (II.2.15) since $W^{(12)}$ is symmetric.

II.3. **Existence of B_2.**

When the existence of B_2 is shown, the transformed Coulomb-Dirac operator up to second order in e^2 takes the form

$$U_2^{-1}U_1^{-1}\; H\; U_1U_2 \;=\; \text{proj}\;(H_0+H_1+H_2)\;+\;\Lambda_+^{(1)}\,\Lambda_+^{(2)}\,V^{(12)}\,\Lambda_+^{(1)}\,\Lambda_+^{(2)}\;+\;R((e^2)^3) \tag{II.3.1}$$

$$H_0 \;=\; \sum_{k=1}^{2} D_0^{(k)}, \quad H_1 \;=\; \sum_{k=1}^{2} V^{(k)}, \quad H_2 \;=\; \sum_{k=1}^{2} C^{(k)} \;+\; C^{(12)}.$$

The existence of $B_2^{(1)}$ and $B_2^{(2)}$ was shown in chapter I and it remains to prove the existence of $B_2^{(12)}$. We start by demonstrating that $B_2^{(12)}$ can be obtained explicitly, and then show the form boundedness of $B_2^{(12)}$. Operator boundedness follows from Lemma I.3.

a) Determination of $B_2^{(12)}$

In order to solve for $B_2^{(12)}$, we apply the unitary transformation $U_0^{'(1)}U_0^{'(2)}$ with $U_0^{'(k)}$ the zero-order single-particle Foldy-Wouthuysen transformation introduced earlier, to the defining equation (II.2.15).
With $S_2^{(12)} := U_0^{'(1)}U_0^{'(2)}\, B_2^{(12)}\, (U_0^{'(1)})^{-1}(U_0^{'(2)})^{-1}$ and the transformation properties of the single-particle operators from Lemma I.7 we obtain

$$U_0^{'(1)}U_0^{'(2)}\,\text{off}\,(C^{(12)})\;(U_0^{'(1)})^{-1}(U_0^{'(2)})^{-1} \;=\; -i\;[(\beta^{(1)}E_p^{(1)}\;+\;\beta^{(2)}E_p^{(2)}), S_2^{(12)}]. \tag{II.3.2}$$

In order to get rid of the matrix-valued operators $\beta^{(k)}$ on the r.h.s. of (II.3.2), the l.h.s. is split into terms of a given symmetry with respect to interchange with $\beta^{(k)}$ (corresponding to the 'even' and 'odd' terms in the single-particle case), $C_{+-}+C_{-+}+C_{--}$, with $\beta^{(1)}C_{+-}=C_{+-}\beta^{(1)}$, $\beta^{(2)}C_{+-}=-C_{+-}\beta^{(2)}$, $\beta^{(1)}C_{-+}=-C_{-+}\beta^{(1)}$, $\beta^{(2)}C_{-+}=C_{-+}\beta^{(2)}$, $\beta^{(1)}C_{--}=-C_{--}\beta^{(1)}$, $\beta^{(2)}C_{--}=-C_{--}\beta^{(2)}$, and $S_2^{(12)} = S_{+-}^{(12)} + S_{-+}^{(12)} + S_{--}^{(12)}$ is split accordingly. Due to the linearity of (II.3.2) this equation can be broken into three decoupled equations for the three contributions of $S_2^{(12)}$.

Using the ΨDO technique (which will be demonstrated in the context of boundedness of $B_2^{(12)}$) to express $S_{+-}^{(12)}$, $S_{-+}^{(12)}$, $S_{--}^{(12)}$ by their respective symbols, the resulting equation for the symbols can be solved explicitly upon reducing the multiplying factor in front of the symbol to a scalar (by suitable multiplication with a linear combination of $\beta^{(1)}$ and $\beta^{(2)}$, using the above symmetry properties as well as $(\beta^{(k)})^2=1$). This proves the uniqueness of $S_2^{(12)}$ and hence of $B_2^{(12)}$ like in the one-particle case.

We add a sketch of the proof that the l.h.s. of (II.3.2) does not contain an even-even contribution (which commutes with both $\beta^{(1)}$ and $\beta^{(2)}$).

First we note that any single-particle 4-spinor in the negative spectral subspace of D_0 can in momentum space be expressed in the form (Rose 1961)

$$\hat{\varphi}_-(\mathbf{p}) \;=\; \frac{1}{\sqrt{2E_p(E_p+m)}}\begin{pmatrix} -\boldsymbol{\sigma}\mathbf{p}\;\hat{v}(\mathbf{p}) \\ (E_p+m)\;\hat{v}(\mathbf{p})\end{pmatrix}, \qquad v\in H_{1/2}(\mathbb{R}^3)\times\mathbb{C}^2 \tag{II.3.3}$$

and for a 4-spinor $\psi_- = \binom{0}{v}$ one has

$$\varphi_- \;=\; U_0^{'-1}\,\psi_- \tag{II.3.4}$$

in complete analogy to $\varphi_+ = U_0^{'-1}\psi_+$ with $\psi_+ = \binom{u}{0}$ and φ_+ in the positive spectral subspace of D_0. Note that in all quantities introduced above a superscript (k) pertaining to particle k has been suppressed.

The absence of an even-even contribution of $U_0^{'(1)}U_0^{'(2)}\mathrm{off}\,(C^{(12)})(U_0^{'(1)})^{-1}(U_0^{'(2)})^{-1}$ means that its expectation value formed with states of the type $\psi_+^{(1)}\psi_+^{(2)},\ \psi_+^{(1)}\psi_-^{(2)},\ \psi_-^{(1)}\psi_+^{(2)},\ \psi_-^{(1)}\psi_-^{(2)}$ vanishes. (In fact, let A be odd with respect to $\beta^{(1)}$. Then $(\psi_+^{(1)}, A\psi_+^{(1)}) = (\beta^{(1)}\psi_+^{(1)}, A\beta^{(1)}\psi_+^{(1)}) = -(\psi_+^{(1)}, (\beta^{(1)})^2\, A\psi_+^{(1)}) = -(\psi_+^{(1)}, A\psi_+^{(1)})$.) However, by means of (II.3.4)ff this is just the expectation value of $\mathrm{off}\,(C^{(12)})$ formed with states of the type φ_{++} (both particles in the positive spectral subspace), $\varphi_{+-},\ \varphi_{-+}$ (one particle in either space) or φ_{--} (both particles in the negative spectral subspace). By definition of the projectors, e.g. $\Lambda_+^{(1)}\Lambda_-^{(2)}\varphi_{+-} = \varphi_{+-},\ \Lambda_+^{(1)}\Lambda_+^{(2)}\varphi_{+-} = \Lambda_-^{(1)}\Lambda_+^{(2)}\varphi_{+-} = \Lambda_-^{(1)}\Lambda_-^{(2)}\varphi_{+-} = 0$, it is easily seen that such expectation values vanish indeed.

This fact establishes the correspondence between the Douglas-Kroll transformation and the Sobolev transformation (proven in section I.3 for single-particle operators) also in the two-particle case.

b) Boundedness of $B_2^{(12)}$

Define the two-particle Fourier transform $\hat{\psi}(\mathbf{p}_1, \mathbf{p}_2)$ of ψ by means of

$$\psi(\mathbf{x}_1, \mathbf{x}_2) \;=\; \frac{1}{(2\pi)^3}\int d\mathbf{p}_1\, d\mathbf{p}_2\; e^{i\mathbf{p}_1 x_1}\; e^{i\mathbf{p}_2 x_2}\;\hat{\psi}(\mathbf{p}_1, \mathbf{p}_2). \tag{II.3.5}$$

Represent the operator $B_2^{(12)}$ by means of its symbol ϕ_{12} via

$$(B_2^{(12)}\psi)(\mathbf{x}_1, \mathbf{x}_2) \;=\; \frac{1}{(2\pi)^3}\int d\mathbf{p}_1\, d\mathbf{p}_2\; e^{i\mathbf{p}_1\mathbf{x}_1}\; e^{i\mathbf{p}_2\mathbf{x}_2}\;\phi_{12}(\mathbf{x}_1, \mathbf{x}_2; \mathbf{p}_1, \mathbf{p}_2)\;\hat{\psi}(\mathbf{p}_1, \mathbf{p}_2)$$

$$=\; \frac{1}{(2\pi)^6}\int d\mathbf{p}_1\, d\mathbf{p}_2\, d\mathbf{s}\, d\mathbf{s}'\; e^{i(\mathbf{p}_1+\mathbf{s})\mathbf{x}_1}\; e^{i(\mathbf{p}_2-\mathbf{s}')\mathbf{x}_2}\;\hat{\phi}_{12}(\mathbf{s}, \mathbf{s}'; \mathbf{p}_1, \mathbf{p}_2)\;\hat{\psi}(\mathbf{p}_1, \mathbf{p}_2) \tag{II.3.6}$$

where we have introduced the Fourier transformed symbol $\hat{\phi}_{12}$. We note that although $V^{(12)}$ depends only on the difference $\mathbf{x}_1 - \mathbf{x}_2$, $B_2^{(12)}$ does not because the single-particle operators in $C^{(12)}$ introduce additional dependences on $\mathbf{x}_1$ respective $\mathbf{x}_2$.

Lemma II.1 (Generalised Lieb and Yau formula).
Let $\psi = \psi(\mathbf{x}_1, \mathbf{x}_2)$ be an antisymmetrised two-particle function. Then for any two-particle essentially self-adjoint operator $A^{(12)}$ with symbol a_{12} one has

$$|(\psi, A^{(12)}\psi)| \;\leq\; c\int d\mathbf{p}_1\, d\mathbf{p}_2\; |\hat{\psi}(\mathbf{p}_1, \mathbf{p}_2)|^2 \cdot I^{(12)}(\mathbf{p}_1, \mathbf{p}_2) \tag{II.3.7}$$

$$I^{(12)}(\mathbf{p}_1, \mathbf{p}_2) := \int d\mathbf{p}_1'\, d\mathbf{p}_2'\; |\hat{a}_{12}(\mathbf{p}_1' - \mathbf{p}_1, \mathbf{p}_2 - \mathbf{p}_2'; \mathbf{p}_1, \mathbf{p}_2)|\; \frac{f(p_1)\, g(p_2)}{f(p_1')\, g(p_2')}$$

where c is a constant and f, g are nonnegative convergence generating functions.

Instead of the factorised form $f(p_1)g(p_2)$ one can also choose a more general form, $f(p_1, p_2)$, with $f \geq 0$.

Proof. With (II.3.5) and (II.3.6) we have

$$(\psi, A^{(12)}\psi) = \frac{1}{(2\pi)^3}\int d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_1' d\mathbf{p}_2' \overline{\hat{\psi}(\mathbf{p}_1,\mathbf{p}_2)}\hat{a}_{12}(\mathbf{p}_1-\mathbf{p}_1', \mathbf{p}_2'-\mathbf{p}_2; \mathbf{p}_1', \mathbf{p}_2')\hat{\psi}(\mathbf{p}_1', \mathbf{p}_2'). \tag{II.3.8}$$

Estimating the integrand of (II.3.8) by means of absolute values of each factor, and subsequently using the Schwarz inequality, one finds

$$|(\psi, A^{(12)}\psi)| \le \tag{II.3.9}$$

$$\frac{1}{(2\pi)^3}\left(\int d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_1' d\mathbf{p}_2' |\hat{\psi}(\mathbf{p}_1,\mathbf{p}_2)|^2 |\hat{a}_{12}(\mathbf{p}_1-\mathbf{p}_1', \mathbf{p}_2'-\mathbf{p}_2, \mathbf{p}_1', \mathbf{p}_2')| \frac{f(p_1)\,g(p_2)}{f(p_1')\,g(p_2')}\right)^{\frac{1}{2}}$$

$$\cdot\left(\int d\mathbf{p}_1\, d\mathbf{p}_2\, d\mathbf{p}_1'\, d\mathbf{p}_2'\, |\hat{\psi}(\mathbf{p}_1', \mathbf{p}_2')|^2\, |\hat{a}_{12}(\mathbf{p}_1-\mathbf{p}_1', \mathbf{p}_2'-\mathbf{p}_2; \mathbf{p}_1', \mathbf{p}_2')|\, \frac{f(p_1')\,g(p_2')}{f(p_1)\,g(p_2)}\right)^{\frac{1}{2}}.$$

From the equality $(A^{(12)}\psi, \psi) = (\psi, A^{(12)}\psi)$ for symmetric operators one derives the relation between the symbol $\hat{a}_{12}$ and its adjoint $\hat{a}_{12}^*$

$$\hat{a}_{12}^*(\mathbf{q}_1, \mathbf{q}_2;\ \mathbf{p}_1, \mathbf{p}_2) \;=\; \hat{a}_{12}(-\mathbf{q}_1, -\mathbf{q}_2; \mathbf{q}_1+\mathbf{p}_1, \mathbf{p}_2-\mathbf{q}_2) \tag{II.3.10}$$

In the second integral of (II.3.9) we interchange $(\mathbf{p}_1, \mathbf{p}_2)$ with $(\mathbf{p}_1', \mathbf{p}_2')$, and in the first integral we use (II.3.10) with $\mathbf{q}_1 := \mathbf{p}_1 - \mathbf{p}_1'$, $\mathbf{q}_2 := \mathbf{p}_2' - \mathbf{p}_2$ and the fact that (like in the one-dimensional case) symbol and its adjoint are in the same symbol class, i.e.

$$|\hat{a}_{12}^*(\mathbf{q}_1, \mathbf{q}_2; \mathbf{p}_1, \mathbf{p}_2)| \;\le\; c_0\, |\hat{a}_{12}(\mathbf{q}_1, \mathbf{q}_2; \mathbf{p}_1, \mathbf{p}_2)|. \tag{II.3.11}$$

Then the inequality (II.3.7) follows immediately with $c := \frac{1}{(2\pi)^3}\, c_0^{\frac{1}{2}}$. ∎

Lemma II.2 (Symbol class of $B_2^{(12)}$)**.**
Let $\hat{w}_{12}$ be the symbol of $W^{(12)}$ which defines the transformation operator $B_2^{(12)}$. Then the symbol $\hat{\phi}_{12}$ of $B_2^{(12)}$ is estimated by

$$|\hat{\phi}_{12}(\mathbf{s}, \mathbf{s}'; \mathbf{p}_1, \mathbf{p}_2)| \;\le\; \frac{c}{s+s'+p_1+p_2+1}\, |\hat{w}_{12}(\mathbf{s}, \mathbf{s}'; \mathbf{p}_1, \mathbf{p}_2)| \tag{II.3.12}$$

with some constant c.

Proof. We first have to rewrite the defining equation (II.2.15) in terms of the respective symbols. From the representation (II.3.6) of $B_2^{(12)}$ we have e.g.

$$(D_0^{(2)} B_2^{(12)}\psi)(\mathbf{x}_1, \mathbf{x}_2) \;=\; \frac{1}{(2\pi)^6}\int d\mathbf{p}_1\, d\mathbf{p}_2\, d\mathbf{s}\, d\mathbf{s}'\; e^{i(\mathbf{p}_1+\mathbf{s})\mathbf{x}_1}\; e^{i(\mathbf{p}_2-\mathbf{s}')\mathbf{x}_2}$$

$$\cdot[\boldsymbol{\alpha}^{(2)}\,(\mathbf{p}_2-\mathbf{s}') \;+\; \beta^{(2)}m]\; \hat{\phi}_{12}(\mathbf{s}, \mathbf{s}'; \mathbf{p}_1, \mathbf{p}_2)\; \hat{\psi}(\mathbf{p}_1, \mathbf{p}_2). \tag{II.3.13}$$

Defining the symbol $\hat{w}_{12}$ by means of an equation corresponding to (II.3.6), (II.2.15) holds if the following equality is satisfied

$$[\boldsymbol{\alpha}^{(1)}\,(\mathbf{p}_1+\mathbf{s}) \;+\; \beta^{(1)}m \;+\boldsymbol{\alpha}^{(2)}\,(\mathbf{p}_2-\mathbf{s}') \;+\; \beta^{(2)}m]\; \hat{\phi}_{12}(\mathbf{s}, \mathbf{s}'; \mathbf{p}_1, \mathbf{p}_2) \tag{II.3.14}$$

$$-\; \hat{\phi}_{12}(\mathbf{s}, \mathbf{s}'; \mathbf{p}_1, \mathbf{p}_2)\; [\boldsymbol{\alpha}^{(1)}\mathbf{p}_1 \;+\; \beta^{(1)}m \;+\; \boldsymbol{\alpha}^{(2)}\mathbf{p}_2 \;+\; \beta^{(2)}m] \;=\; i\, \hat{w}_{12}(\mathbf{s}, \mathbf{s}'; \mathbf{p}_1, \mathbf{p}_2).$$

From this equation it follows that for $p_1 \to 0$, $p_2 \to 0$, $s \to 0$ or $s' \to 0$, the behaviour of $\hat{\phi}_{12}$ is that of $\hat{w}_{12}$, while there occurs an extra power of p_1^{-1}, p_2^{-1}, s^{-1} or s'^{-1}, respectively, for $p_1 \to \infty$, $p_2 \to \infty$, $s \to \infty$ or $s' \to \infty$, respectively. This leads to the estimate (II.3.12). ∎

Recalling that $W^{(12)} = \mathrm{off}\,(C^{(12)})$, it follows from (II.2.13) that, apart from factors $\Lambda_\pm$, $\hat{w}_{12}$ is determined from the commutators $[V^{(12)}, B_1^{(k)}]$ and $[F_0^{(k)}, V^{(12)}]$. In the context of boundedness of $B_2^{(12)}$, these additional factors $\Lambda_\pm$ can be disregarded since they are bounded multiplication operators in momentum space. We start by showing that $F_0^{(k)}$ is in the same symbol class as $B_1^{(k)}$ such that it will be sufficient to consider only the commutator $[V^{(12)}, B_1^{(k)}]$.

Lemma II.3 (Symbol class of F_0).
Let F_0 be defined by

$$F_0 \;=\; -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\eta\, \frac{1}{D_0+i\eta}\, V\, \frac{1}{D_0+i\eta} \tag{II.3.15}$$

with $V = -\gamma/x$ the Coulomb field, and let f_0 be its symbol. Then one has the following estimate

$$|\hat{f}_0(\mathbf{q},\mathbf{p})| \;\le\; \gamma\,\frac{c}{q}\,\frac{1}{(q+p+1)^2}. \tag{II.3.16}$$

Proof. We introduce the Fourier representation of V and of the single-particle function φ to write

$$(F_0\varphi)(\mathbf{x}) \;=\; \frac{\gamma}{(2\pi)^{5/2}}\int_{-\infty}^{\infty} d\eta\, \frac{1}{D_0+i\eta}\int d\mathbf{q}\, e^{i\mathbf{qx}}\,\frac{1}{2\pi^2 q^2}\,\frac{1}{D_0+i\eta}\int d\mathbf{p}\, e^{i\mathbf{px}}\,\hat{\varphi}(\mathbf{p}). \tag{II.3.17}$$

Using that $\dfrac{1}{D_0+i\eta}\,e^{i\mathbf{px}} = \dfrac{D_0-i\eta}{D_0^2+\eta^2}\,e^{i\mathbf{px}} = \dfrac{D_0-i\eta}{E_p^2+\eta^2}\,e^{i\mathbf{px}}$ with $D_0(\mathbf{p}) = \boldsymbol{\alpha}\mathbf{p}+\beta m$, and that the odd terms in η vanish upon integration, the theorem of residues can be applied to evaluate the η-integral. The contour is closed over the upper half plane where the two poles at $\eta = iE_p$ and $\eta = iE_{|\mathbf{p}+\mathbf{q}|}$ have to be considered. This leads to

$$\int_{-\infty}^{\infty} d\eta\, \frac{D_0(\mathbf{q}+\mathbf{p})D_0(\mathbf{p})-\eta^2}{(E_{|\mathbf{q}+\mathbf{p}|}^2+\eta^2)(E_p^2+\eta^2)}$$

$$= \frac{\pi}{E_p^2-E_{|\mathbf{q}+\mathbf{p}|}^2}\left(\frac{D_0(\mathbf{q}+\mathbf{p})D_0(\mathbf{p})+E_{|\mathbf{q}+\mathbf{p}|}^2}{E_{|\mathbf{q}+\mathbf{p}|}} - \frac{D_0(\mathbf{q}+\mathbf{p})D_0(\mathbf{p})+E_p^2}{E_p}\right)$$

$$= -\frac{\pi}{E_p+E_{|\mathbf{q}+\mathbf{p}|}}\,(1\;-\;\tilde{D}_0(\mathbf{q}+\mathbf{p})\,\tilde{D}_0(\mathbf{p})) \tag{II.3.18}$$

with $\tilde{D}_0 := D_0/|D_0|$ as before. Comparing with the standard definition (I.1.13) of F_0 in terms of its symbol f_0, its momentum representation is extracted from (II.3.17),

$$\hat{f}_0(\mathbf{q},\mathbf{p}) \;=\; -\frac{\gamma}{\sqrt{2\pi}}\,\frac{1}{q^2}\,\frac{1}{E_p+E_{|\mathbf{q}+\mathbf{p}|}}\,(1\;-\;\tilde{D}_0(\mathbf{q}+\mathbf{p})\,\tilde{D}_0(\mathbf{p})), \tag{II.3.19}$$

which shows that the symbol (and hence the kernel) of F_0 has a negative (or zero) real part for all $\mathbf{q},\mathbf{p}\in\mathbb{R}^3$. Note that $\hat{f}_0$ satisfies the condition (I.1.15) for self-adjointness of F_0. From Lemma I.5 it follows that there is a simple relation between $\hat{f}_0$ and the symbol $\hat{\phi}_1$ of B_1,

$$\hat{f}_0(\mathbf{q},\mathbf{p}) \;=\; -i\,\tilde{D}_0(\mathbf{q}+\mathbf{p})\,\hat{\phi}_1(\mathbf{q},\mathbf{p}) \tag{II.3.20}$$

such that Lemma II.3 is a consequence of Lemma I.5. ∎

From (II.3.15) it is also easily seen that F_0 is a self-adjoint operator since the integration region is symmetric in η. Thus we derive from (II.3.20) the operator relations

$$\begin{aligned} F_0 &= -i\,\tilde{D}_0\,B_1 \;=\; i\,B_1\,\tilde{D}_0 \\ B_1 &= i\,\tilde{D}_0\,F_0 \;=\; -i\,F_0\,\tilde{D}_0 \end{aligned} \tag{II.3.21}$$

where the second line is obtained from the first one upon multiplication by $i\tilde{D}_0$.

Now we aim at expressing the symbol of $B_2^{(12)}$ by the symbols of the commutator $[V^{(12)}, B_1^{(k)}]$. Let $w_a^{(12)}$ be the symbol of $V^{(12)}B_1^{(1)}$ and $w_b^{(12)}$ the one of $B_1^{(1)}V^{(12)}$.

Due to the antisymmetry of ψ and the invariance of $V^{(12)}$ upon particle exchange, one has

$$(\psi, (V^{(12)} B_1^{(2)} \; - B_1^{(2)} V^{(12)})\; \psi) \; = \; (\psi, (V^{(12)} B_1^{(1)} \; - B_1^{(1)} V^{(12)})\; \psi) \tag{II.3.22}$$

such that one can estimate from (II.3.12)

$$\left|\hat{\phi}_{12}(\mathbf{s},\mathbf{s}';\mathbf{p}_1,\mathbf{p}_2)\right| \leq \frac{c_1}{s+s'+p_1+p_2+1} \left\{|\hat{w}_a^{(12)}(\mathbf{s},\mathbf{s}';\mathbf{p}_1,\mathbf{p}_2)|+|\hat{w}_b^{(12)}(\mathbf{s},\mathbf{s}';\mathbf{p}_1,\mathbf{p}_2)|\right\} \tag{II.3.23}$$

with a suitable constant c_1.

We proceed by calculating $\hat{w}_a^{(12)}$ and $\hat{w}_b^{(12)}$. With

$$\chi(\mathbf{x}_1,\mathbf{x}_2) := \; (B_1^{(1)}\psi)(\mathbf{x}_1,\mathbf{x}_2) \tag{II.3.24}$$

$$= \; \frac{1}{(2\pi)^3} \int d\mathbf{p}_1' \; d\mathbf{s}' \; e^{i\mathbf{p}_1'\mathbf{x}_1} e^{i\mathbf{s}'\mathbf{x}_1} \; \hat{\phi}_1^{(1)}(\mathbf{s}',\mathbf{p}_1') \; \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\mathbf{p}_2' \; e^{i\mathbf{p}_2'\mathbf{x}_2} \; \hat{\psi}(\mathbf{p}_1',\mathbf{p}_2')$$

and its momentum representation

$$\hat{\chi}(\mathbf{p}_1,\mathbf{p}_2) \; = \; \frac{1}{(2\pi)^3} \int d\mathbf{x}_1 \; d\mathbf{x}_2 \; e^{-i\mathbf{p}_1\mathbf{x}_1} e^{-i\mathbf{p}_2\mathbf{x}_2} \; \chi(\mathbf{x}_1,\mathbf{x}_2) \tag{II.3.25}$$

$$= \; \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\mathbf{s}' \; \hat{\phi}_1^{(1)}(\mathbf{s}',\mathbf{p}_1-\mathbf{s}') \; \hat{\psi}(\mathbf{p}_1-\mathbf{s}',\mathbf{p}_2)$$

we get, following (II.3.6) and subsequently making the variable transforms $\mathbf{p}_1 - \mathbf{s}' \mapsto \mathbf{p}_1$, $\mathbf{s}+\mathbf{s}' = \mathbf{s}''$ (finally replacing $\mathbf{s} \mapsto \mathbf{s}'$, $\mathbf{s}'' \mapsto \mathbf{s}$),

$$(V^{(12)} \underbrace{B_1^{(1)}\psi}_{\chi}(\mathbf{x}_1,\mathbf{x}_2) = \frac{1}{(2\pi)^3} \frac{1}{2\pi^2} \int d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{s} \frac{e^2}{s^2} e^{i\mathbf{p}_1\mathbf{x}_1} e^{i\mathbf{p}_2\mathbf{x}_2} e^{i\mathbf{s}(\mathbf{x}_1-\mathbf{x}_2)} \hat{\chi}(\mathbf{p}_1,\mathbf{p}_2)$$

$$= \; \frac{e^2}{(2\pi)^6} \sqrt{\frac{2}{\pi}} \int d\mathbf{p}_1 \; d\mathbf{p}_2 \; d\mathbf{s} \; d\mathbf{s}' \; e^{i(\mathbf{p}_1+\mathbf{s})\mathbf{x}_1} e^{i(\mathbf{p}_2-\mathbf{s}')\mathbf{x}_2} \; \frac{e^2}{s'^2} \; \hat{\phi}_1^{(1)}(\mathbf{s}-\mathbf{s}',\mathbf{p}_1) \; \hat{\psi}(\mathbf{p}_1,\mathbf{p}_2). \tag{II.3.26}$$

Comparing with (II.3.6) we can extract the symbol of $V^{(12)}B_1^{(1)}$,

$$\hat{w_a}^{(12)}(\mathbf{s},\mathbf{s}';\mathbf{p}_1,\mathbf{p}_2) \; = \; \sqrt{\frac{2}{\pi}} \; \frac{e^2}{s'^2} \; \hat{\phi}_1^{(1)}(\mathbf{s}-\mathbf{s}',\mathbf{p}_1). \tag{II.3.27}$$

Similarly,

$$(B_1^{(1)} \; V^{(12)} \; \psi)(\mathbf{x}_1,\mathbf{x}_2) \; = \; \frac{1}{(2\pi)^6} \int d\mathbf{p}_1 \; d\mathbf{p}_2 \; d\mathbf{s} \, d\mathbf{s}' \; e^{i(\mathbf{p}_1+\mathbf{s})\mathbf{x}_1} e^{i(\mathbf{p}_2-\mathbf{s}')\mathbf{x}_2}$$

$$\cdot \sqrt{\frac{2}{\pi}} \; \hat{\phi}_1^{(1)}(\mathbf{s}-\mathbf{s}',\mathbf{p}_1+\mathbf{s}') \; \frac{e^2}{s'^2} \; \hat{\psi}(\mathbf{p}_1,\mathbf{p}_2) \tag{II.3.28}$$

whence

$$\hat{w}_b^{(12)}(\mathbf{s},\mathbf{s}';\mathbf{p}_1,\mathbf{p}_2) \; = \; \sqrt{\frac{2}{\pi}} \; \frac{e^2}{s'^2} \; \hat{\phi}_1^{(1)}(\mathbf{s}-\mathbf{s}',\mathbf{p}_1+\mathbf{s}'). \tag{II.3.29}$$

In order to prove the form boundedness of $B_2^{(12)}$, we apply the generalised Lieb and Yau formula (II.3.7), such that with the estimate (II.3.23),

$$|(\psi, B_2^{(12)} \; \psi)| \; \leq \; c \int d\mathbf{p}_1 \; d\mathbf{p}_2 \; |\hat{\psi}(\mathbf{p}_1,\mathbf{p}_2)| \cdot I^{(12)}(\mathbf{p}_1,\mathbf{p}_2)$$

$$I^{(12)}(\mathbf{p}_1,\mathbf{p}_2) \; \leq \; c_1 \int d\mathbf{p}_1' \; d\mathbf{p}_2' \; \frac{f(p_1)\, g(p_2)}{f(p_1')\, g(p_2')} \; \frac{1}{|\mathbf{p}_1-\mathbf{p}_1'|+|\mathbf{p}_2-\mathbf{p}_2'|+p_1+p_2+1} \tag{II.3.30}$$

$$\cdot \, e^2 \sqrt{\frac{2}{\pi}} \left\{ \frac{1}{|\mathbf{p}_2-\mathbf{p}_2'|^2} |\hat{\phi}_1^{(1)}(\mathbf{p}_1'-\mathbf{p}_1-\mathbf{p}_2+\mathbf{p}_2',\mathbf{p}_1)| \right.$$

$$+\ \frac{1}{|\mathbf{p}_2-\mathbf{p}_2'|^2}\ |\hat{\phi}_1^{(1)}(\mathbf{p}_1'-\mathbf{p}_1-\mathbf{p}_2+\mathbf{p}_2',\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_2')|\Big\}.$$

We make the substitution $\mathbf{p}_2'-\mathbf{p}_2=:\mathbf{q}$ for $\mathbf{p}_2'$ and estimate $(|\mathbf{p}_1-\mathbf{p}_1'|+|\mathbf{p}_2-\mathbf{p}_2'|+p_1+p_2+1)^{-1}\ \le c\,p_2'^{-1}$. Then with the estimate (I.2.17) for $\hat{\phi}_1^{(1)}$,

$$I^{(12)}(\mathbf{p}_1,\mathbf{p}_2)\ \le\ C\int d\mathbf{q}\ \frac{1}{|\mathbf{q}+\mathbf{p}_2|}\ \frac{1}{q^2}\ \frac{g(p_2)}{g(|\mathbf{q}+\mathbf{p}_2|)}\int d\mathbf{p}_1'\ \frac{\tilde{c}}{|\mathbf{p}_1'-\mathbf{p}_1+\mathbf{q}|} \tag{II.3.31}$$

$$\cdot\left(\frac{1}{(|\mathbf{p}_1'-\mathbf{p}_1+\mathbf{q}|+p_1+1)^2}\ +\ \frac{1}{(|\mathbf{p}_1'-\mathbf{p}_1+\mathbf{q}|+|\mathbf{p}_1-\mathbf{q}|+1)^2}\right)\frac{f(p_1)}{f(p_1')}.$$

Choosing $f(p)=p$ and keeping $\boldsymbol{\xi}:=\mathbf{p}_1-\mathbf{q}$ constant, the first $\mathbf{p}_1'$-integral reduces to

$$I_\xi\ :=\ \int d\mathbf{p}_1'\ \frac{\tilde{c}}{|\mathbf{p}_1'-\boldsymbol{\xi}|}\ \frac{1}{(|\mathbf{p}_1'-\boldsymbol{\xi}|+p_1+1)^2}\ \frac{p_1}{p_1'}. \tag{II.3.32}$$

The angular integration is done with the help of Appendix A, resulting in

$$I_\xi\ =\ 2\pi\,\tilde{c}\ \frac{p_1}{\xi}\int_0^\infty dp_1'\ \left(\frac{1}{|p_1'-\xi|+p_1+1}\ -\ \frac{1}{p_1'+\xi+p_1+1}\right)$$

$$=\ 4\pi\,\tilde{c}\ \frac{p_1}{\xi}\ \ln\frac{\xi+p_1+1}{p_1+1}\ =\ 4\pi\,\tilde{c}\ \frac{p_1}{|\mathbf{p}_1-\mathbf{q}|}\ \ln\frac{|\mathbf{p}_1-\mathbf{q}|+p_1+1}{p_1+1} \tag{II.3.33}$$

In order to prove that I_ξ is bounded, i.e. $I_\xi\le C_0<\infty$ for all $\mathbf{q},\mathbf{p}_1\in\mathbb{R}^3$, we first investigate the case $\xi=0$ (i.e. $\mathbf{p}_1=\mathbf{q}$). From (II.3.32),

$$I_0\ =\ \int d\mathbf{p}_1'\ \frac{\tilde{c}}{p_1'}\ \frac{1}{(p_1'+p_1+1)^2}\ \frac{p_1}{p_1'}\ =\ 4\pi\,\tilde{c}\int_0^\infty dp_1'\ \frac{p_1}{(p_1'+p_1+1)^2}$$

$$=\ 4\pi\,\tilde{c}\ \frac{p_1}{p_1+1}\ <\infty. \tag{II.3.34}$$

If $\xi\neq 0$, one finds by inspection of (II.3.33) that $I_\xi\to 0$ for $p_1\to 0$ or $q\to\infty$ while $I_\xi<\infty$ for $q\to 0$ or $p_1\to\infty$. Since for $\xi\neq 0$, I_ξ is a continuous function of both variables in $\mathbb{R}^3\times\mathbb{R}^3$, this proves its boundedness.

The second $\mathbf{p}_1'$-integral in (II.3.31) results in $4\pi\tilde{c}\ \ln\frac{2\xi+1}{\xi+1}$ in place of I_ξ, which is also bounded. Choosing $g(p)=p$, we have thus

$$I^{(12)}(\mathbf{p}_1,\mathbf{p}_2)\ \le\ C'\int d\mathbf{q}\ \frac{1}{q^2}\ \frac{p_2}{|\mathbf{q}+\mathbf{p}_2|^2}\ =\ C'\,\pi^3\ <\infty \tag{II.3.35}$$

where Appendix A was used. Therefore,

$$|(\psi,B_2^{(12)}\psi)|\ \le\ \tilde{C}\ (\psi,\psi). \tag{II.3.36}$$

II.4. **The transformed Coulomb-Dirac operator.**

We shall restrict $H^{(n)}$ of section II.2 to the two-particle positive spectral subspace $\mathcal{H}_{+,2}$. Due to the properties (II.2.1), only the first term of $H^{(n)}$ survives in the expectation value. Let us concentrate on that contribution to $H^{(n)}$ for $n=2$, which affects both particles simultaneously. From (II.3.1) and (II.2.13) for $\psi\in\mathcal{H}_{+,2}$ with the property $\Lambda_+^{(1)}\psi=\psi=\Lambda_+^{(2)}\psi$, one obtains

$$(\psi,H_{12}\,\psi):=\ (\psi,\Lambda_+^{(1)}\Lambda_+^{(2)}\,V^{(12)}\,\Lambda_+^{(1)}\Lambda_+^{(2)}\ \psi)\ +\ (\psi,C^{(12)}\,\psi)$$

$$=\ (\psi,V^{(12)}\,\psi)\ +\ i\,(\psi,\sum_{k=1}^{2}(V^{(12)}\Lambda_+^{(1)}\Lambda_+^{(2)}\,B_1^{(k)}\ -\ B_1^{(k)}\,\Lambda_+^{(1)}\Lambda_+^{(2)}V^{(12)})\,\psi) \tag{II.4.1}$$

$$+\ (\psi,\ [\,(F_0^{(1)}\ +\ F_0^{(2)})\,V^{(12)}\ +\ V^{(12)}\,(F_0^{(1)}\ +\ F_0^{(2)})\,]\,\psi)$$

Due to the exchange antisymmetry of ψ, an equivalent representation of (II.4.1) is

$$(\psi, H_{12}\,\psi) \;=\; (\psi, V^{(12)}\,\psi) \;+\; 2i\,(\psi, (V^{(12)}\Lambda_+^{(1)}\,B_1^{(1)} \;-\; B_1^{(1)}\,\Lambda_+^{(1)}V^{(12)})\,\psi)$$
$$+\,2\,(\psi,\,(F_0^{(1)}V^{(12)} \;+\; V^{(12)}F_0^{(1)})\,\psi), \tag{II.4.2}$$

which is more convenient for mathematical analysis (although in applications an operator, which is symmetric in both particles, is usually prefered).

The second-order term is further simplified by means of (II.3.21),

$$\begin{aligned}(\psi, C^{(12)}\,\psi) \;&=\; 2\,(\psi,\;(V^{(12)}\,\Lambda_-^{(1)}\,F_0^{(1)} \;+\; F_0^{(1)}\,\Lambda_-^{(1)}\,V^{(12)})\,\psi)\\ &=\; 2\,(\psi,\,i\,(V^{(12)}\,\Lambda_-^{(1)}\,B_1^{(1)} \;-\; B_1^{(1)}\,\Lambda_-^{(1)}\,V^{(12)})\,\psi).\end{aligned} \tag{II.4.3}$$

Collecting results and using (I.3.24) for the single-particle contribution, the total transformed two-particle operator acting on $\mathcal{H}_{+,2}$ can be reduced to the following expression

$$H^{(2)} \;=\; \sum_{k=1}^{2}\left(D_0^{(k)} \;+\; V^{(k)} \;+\; \frac{i}{2}\,[W_1^{(k)}, B_1^{(k)}]\right) \;+\; V^{(12)} \;+\; C^{(12)} \tag{II.4.4}$$

$$C^{(12)} \;=\; \sum_{k=1}^{2}\left(V^{(12)}\,\Lambda_-^{(k)}\,F_0^{(k)} \;+\; F_0^{(k)}\,\Lambda_-^{(k)}\,V^{(12)}\right),$$

where we have again used the symmetrised form of the second-order two-particle term $C^{(12)}$. In order to derive its explicit form, we recall

$$\Lambda_-^{(k)} = \frac{1}{2}\,(1-\tilde{D}_0^{(k)}),\quad \hat{\phi}_1^{(1)}(\mathbf{q},\mathbf{p}) = -i\,\frac{\gamma}{\sqrt{2\pi}}\,\frac{1}{q^2}\,\frac{1}{E_{|\mathbf{q}+\mathbf{p}|}+E_p}\,(\tilde{D}_0^{(1)}(\mathbf{q}+\mathbf{p})-\tilde{D}_0^{(1)}(\mathbf{p})) \tag{II.4.5}$$

and (II.3.24), (II.3.26) to obtain

$$(\psi, V^{(12)}\Lambda_-^{(1)}\,B_1^{(1)}\,\psi) \;=\; (V^{(12)}\,\psi, \Lambda_-^{(1)}\,B_1^{(1)}\,\psi)$$
$$=\;\frac{e^2}{(2\pi)^{\frac{3}{2}}\cdot 4\pi^2}\int d\mathbf{p}_1\,d\mathbf{p}_2\,d\mathbf{p}_1'\,d\mathbf{p}_2'\,\overline{\hat{\psi}(\mathbf{p}_1,\mathbf{p}_2)}\,\frac{1}{|\mathbf{p}_2-\mathbf{p}_2'|^2}\,(1\;-\;\tilde{D}_0^{(1)}(\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1))$$
$$\cdot\hat{\phi}_1^{(1)}(\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1-\mathbf{p}_1',\mathbf{p}_1')\,\hat{\psi}(\mathbf{p}_1',\mathbf{p}_2') \tag{II.4.6}$$

and

$$(\psi, B_1^{(1)}\Lambda_-^{(1)}V^{(12)}\,\psi) \;=\; (\Lambda_-^{(1)}B_1^{(1)}\,\psi, V^{(12)}\,\psi)$$
$$=\;\frac{e^2}{(2\pi)^{\frac{3}{2}}\cdot 4\pi^2}\int d\mathbf{p}_1\,d\mathbf{p}_2\,d\mathbf{p}_1'\,d\mathbf{p}_2'\,\overline{\hat{\psi}(\mathbf{p}_1,\mathbf{p}_2)}\,\hat{\phi}_1^{(1)*}(\mathbf{p}_2'-\mathbf{p}_2+\mathbf{p}_1'-\mathbf{p}_1,\mathbf{p}_1)$$
$$\cdot(1\;-\;\tilde{D}_0^{(1)}(\mathbf{p}_2'-\mathbf{p}_2+\mathbf{p}_1'))\,\frac{1}{|\mathbf{p}_2'-\mathbf{p}_2|^2}\,\hat{\psi}(\mathbf{p}_1',\mathbf{p}_2'). \tag{II.4.7}$$

We define the kernel $k_{A^{(12)}}$ of a two-particle operator $A^{(12)}$ by means of

$$(\psi, A^{(12)}\psi) \;=\; \int d\mathbf{p}_1\,d\mathbf{p}_2\,\overline{\hat{\psi}(\mathbf{p}_1,\mathbf{p}_2)}\int d\mathbf{p}_1'\,d\mathbf{p}_2'\,k_{A^{(12)}}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2')\,\hat{\psi}(\mathbf{p}_1',\mathbf{p}_2') \tag{II.4.8}$$

which is related to the Fourier transformed symbol $\hat{a}_{12}$ of $A^{(12)}$ from (II.3.8) by means of

$$k_{A^{(12)}}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2') \;=\; \frac{1}{(2\pi)^3}\,\hat{a}_{12}(\mathbf{p}_1-\mathbf{p}_1',\mathbf{p}_2'-\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2'). \tag{II.4.9}$$

Then

$$k_{C^{(12)}}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2') \;=\; -\frac{2\gamma e^2}{(2\pi)^4}\,\frac{1}{|\mathbf{p}_2-\mathbf{p}_2'|^2}\,\frac{1}{|\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1-\mathbf{p}_1'|^2}$$

$$\cdot \left\{ \frac{1}{E_{|\mathbf{p}_2 - \mathbf{p}_2' + \mathbf{p}_1|} + E_{p_1'}} \, (1 - \tilde{D}_0^{(1)}(\mathbf{p}_2 - \mathbf{p}_2' + \mathbf{p}_1))\, (1 + \tilde{D}_0^{(1)}(\mathbf{p}_1')) \right.$$

$$\left. + \frac{1}{E_{p_1} + E_{|\mathbf{p}_2' - \mathbf{p}_2 + \mathbf{p}_1'|}} \, (1 + \tilde{D}_0^{(1)}(\mathbf{p}_1))\, (1 - \tilde{D}_0^{(1)}(\mathbf{p}_2' - \mathbf{p}_2 + \mathbf{p}_1')) \right\}. \qquad \text{(II.4.10)}$$

Since $\|\tilde{D}_0^{(1)}\| = 1,$ the expression in curly brackets is a matrix-valued function with a nonnegative real part, and therefore Re $k_{C^{12}} \leq 0$ for all $\mathbf{p}_k, \mathbf{p}_k' \in \mathbb{R}^3,\; k = 1, 2.$

For the contribution to H_{12} which is linear in e^2 one gets with (II.3.5) and (II.3.26)

$$k_{V^{(12)}}(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p}_1', \mathbf{p}_2') \;=\; \frac{1}{2\pi^2}\, \frac{e^2}{|\mathbf{p}_2' - \mathbf{p}_2|^2}\, \delta(\mathbf{p}_2' - \mathbf{p}_2 + \mathbf{p}_1' - \mathbf{p}_1) \;\geq\; 0. \qquad \text{(II.4.11)}$$

Note that the singularities of the kernels of $C^{(12)}$ and $V^{(12)}$ coincide, but they are of different type.

II.5. **Properties of the transformed Coulomb-Dirac operator.**

Having established the explicit form of the transformed two-particle Coulomb-Dirac operator up to second order in the coupling constant e^2, we will now show the subordinacy of the interaction terms with respect to the kinetic energy, and ultimately the positivity of the transformed operator. Of course, both properties will only be valid for not too large central potentials.

a) p-form boundedness of $C^{(12)}$

Lemma II.4 (*p*-form boundedness of second-order potential)**.**
Let $C_1^{(12)} := V^{(12)} \Lambda_-^{(1)} F_0^{(1)} + F_0^{(1)} \Lambda_-^{(1)} V^{(12)}$ *with* $V^{(12)}$ *the electron-electron Coulomb interaction and* $F_0^{(1)}$ *the first-order expansion term of the projector* $P_+^{(1)}$*, defined in (II.2.9). Then for* $\psi \in \mathcal{H}_{+,2}$,

$$|(\psi, C_1^{(12)}\, \psi)| \;\leq\; \gamma e^2\, \frac{\pi^2}{4}\, (\psi, p_1\, \psi) \;\leq\; \gamma\, e^2\, \frac{\pi^2}{4}\, (\psi, E_{p_1}\, \psi) \qquad \text{(II.5.1)}$$

with form bound $\gamma e^2 \frac{\pi^2}{4} < 1$ *for* $\gamma e^2 < 0.405$ *corresponding to* $Z \leq 55/e^2$.

Since ψ is antisymmetric with respect to particle exchange, one can replace $(\psi, p_1 \psi)$ by $\frac{1}{2}\, (\psi, (p_1 + p_2)\, \psi)$ on the r.h.s. of (II.5.1), such that for $C^{(12)}$ from (II.4.3), Lemma II.4 gives

$$|(\psi, C^{(12)}\, \psi)| \;\leq\; \gamma e^2\, \frac{\pi^2}{4}\, (\psi, (p_1 + p_2)\, \psi) \;\leq\; \gamma\, e^2\, \frac{\pi^2}{4}\, (\psi, (E_{p_1} + E_{p_2})\, \psi). \quad \text{(II.5.2)}$$

Proof. Using the generalised Lieb and Yau formula (Lemma II.1), we have

$$|(\psi, C_1^{(12)}\, \psi)| \;=\; |(\psi, \frac{1}{2}\, C^{(12)}\, \psi)|$$

$$\leq \int d\mathbf{p}_1\, d\mathbf{p}_2\, d\mathbf{p}_1'\, d\mathbf{p}_2'\, |\hat{\psi}(\mathbf{p}_1, \mathbf{p}_2)|\, \frac{1}{2}\, |k_{c^{(12)}}(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p}_1', \mathbf{p}_2')|\, |\hat{\psi}(\mathbf{p}_1', \mathbf{p}_2')|$$

$$\leq \int d\mathbf{p}_1\, d\mathbf{p}_2\, |\hat{\psi}(\mathbf{p}_1, \mathbf{p}_2)|^2 \cdot J_0(\mathbf{p}_1, \mathbf{p}_2) \qquad \text{(II.5.3)}$$

$$J_0(\mathbf{p}_1, \mathbf{p}_2) := \frac{1}{2} \int d\mathbf{p}_1'\, d\mathbf{p}_2'\, |k_{C^{(12)}}(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p}_1', \mathbf{p}_2')|\, \frac{f(p_1)}{f(p_1')}\, \frac{g(p_2)}{g(p_2')}.$$

For the convergence generating functions we choose $g = 1$ and $f(p) = p^2$. Moreover, one has

$$|1 \pm \tilde{D}_0| \;\leq\; 1 \,+\, |\tilde{D}_0| \;=\; 2. \tag{II.5.4}$$

Hence, inserting the explicit form (II.4.10) for the kernel of $C^{(12)}$, it follows

$$J_0(\mathbf{p}_1,\mathbf{p}_2) \;\leq\; \frac{\gamma e^2}{(2\pi)^4} \int d\mathbf{p}_1'\, d\mathbf{p}_2' \,\frac{1}{|\mathbf{p}_2'-\mathbf{p}_2|^2}\, \frac{1}{|\mathbf{p}_2'-\mathbf{p}_2+\mathbf{p}_1'-\mathbf{p}_1|^2}$$

$$\cdot\, 4 \left\{ \frac{1}{E_{|\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1|} + E_{p_1'}} \,+\, \frac{1}{E_{|\mathbf{p}_2'-\mathbf{p}_2+\mathbf{p}_1'|} + E_{p_1}} \right\} \cdot \frac{p_1^2}{p_1'^2}. \tag{II.5.5}$$

Since the integrand is a nonnegative function, one can estimate the energy denominators by their value for mass $m = 0$. We denote the two summands of J_0 by J_a and J_b, respectively,

$$J_0(\mathbf{p}_1,\mathbf{p}_2) \;=\; 4\,\frac{\gamma e^2}{(2\pi)^4}\,(J_a \,+\, J_b)(\mathbf{p}_1,\mathbf{p}_2) \tag{II.5.6}$$

and replace $\mathbf{p}_2'$ by $\boldsymbol{\xi}_2 := \mathbf{p}_2' - \mathbf{p}_2 - \mathbf{p}_1$ in J_a. Then

$$J_a(\mathbf{p}_1,\mathbf{p}_2) \;\leq\; \int d\mathbf{p}_1'\, d\mathbf{p}_2'\, \frac{1}{|\mathbf{p}_2'-\mathbf{p}_2|^2}\, \frac{1}{|\mathbf{p}_2'-\mathbf{p}_2+\mathbf{p}_1'-\mathbf{p}_1|^2}\, \frac{1}{|\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1| \,+ p_1'}\, \frac{p_1^2}{p_1'^2}$$

$$= \; p_1^2 \int d\boldsymbol{\xi}_2\, \frac{1}{|\boldsymbol{\xi}_2+\mathbf{p}_1|^2} \int \frac{d\mathbf{p}_1'}{p_1'^2}\, \frac{1}{\xi_2+p_1'}\, \frac{1}{|\boldsymbol{\xi}_2+\mathbf{p}_1'|^2}. \tag{II.5.7}$$

The second integral is readily evaluated with the help of Appendix A, yielding $\pi^3/(2\xi_2^2)$. Again using Appendix A for the remaining integral, one obtains the estimate for J_a,

$$J_a(\mathbf{p}_1,\mathbf{p}_2) \;\leq\; \frac{\pi^6}{2}\, p_1. \tag{II.5.8}$$

In the second contribution to J_0 one makes the substitutions $\mathbf{q}_2' := \mathbf{p}_2' - \mathbf{p}_2$ for $\mathbf{p}_2'$ and subsequently $\mathbf{q}_1 := \mathbf{q}_2' + \mathbf{p}_1'$ for $\mathbf{p}_1'$. Then

$$J_b(\mathbf{p}_1,\mathbf{p}_2) \;\leq\; \int d\mathbf{q}_1\, \frac{1}{|\mathbf{q}_1-\mathbf{p}_1|^2}\, \frac{p_1^2}{q_1+p_1} \int \frac{d\mathbf{q}_2'}{q_2'^2}\, \frac{1}{|\mathbf{q}_2'-\mathbf{q}_1|^2} \tag{II.5.9}$$

and the two integrals involved are the same as for J_a. Hence, $J_b(\mathbf{p}_1,\mathbf{p}_2)$ is also estimated by the r.h.s. of (II.5.8). Insertion into (II.5.3) yields

$$|(\psi, C_1^{(12)}\psi)| \;\leq\; \int d\mathbf{p}_1\, d\mathbf{p}_2\, |\hat{\psi}(\mathbf{p}_1,\mathbf{p}_2)|^2 \cdot \frac{4\gamma e^2}{(2\pi)^4} \cdot \pi^6\, p_1 \tag{II.5.10}$$

which, since $p_1 \leq E_{p_1}$, is the assertion of Lemma II.4. ■

b) Subordinacy of $C^{(12)}$

We show that for sufficiently small potential strength, the second-order term $C^{(12)}$ can be controlled by the electron-electron potential $V^{(12)}$. Also, considering the limit of an infinite translation, $C^{(12)}$ is subordinate to $V^{(12)}$ in the form sense. As a consequence, the form sum of $V^{(12)}$ and $C^{(12)}$ is positive (corresponding to a repulsive total two-particle potential).

Proposition II.2 (Subdominance of second-order potential).
Let $C^{(12)}$ be the second-order two-particle potential and $V^{(12)} = e^2/|\mathbf{x}_1 - \mathbf{x}_2|$. Then for $\psi \in \mathcal{H}_{+,2}$,

(i)

$$|(\psi, C^{(12)}\,\psi)| \;\leq\; c\,\|V^{(12)}\,\psi\| \,\cdot \|\psi\| \tag{II.5.11}$$

with $c < 1$ for $\gamma < \frac{\pi}{\pi^2-4} = 0.535$ $(Z \leq 73)$.

(ii)

$$|(\psi, C^{(12)}\,\psi)| \;\leq\; \pi\, C\, \gamma\; (\psi, V^{(12)}\,\psi) \tag{II.5.12}$$

with relative form bound smaller than one for $\gamma < \frac{1}{\pi C}$, C *being a constant of order unity.*

If for the proof of (i), the same estimates are used as for (ii), one gets $c < 1$ if $\gamma < 1/\pi \;\; (Z \leq 43)$, corresponding to $C = 1$.

Proof of (i).
With the definition of $C^{(12)}$ we have

$$|(\psi, C^{(12)}\,\psi)| \;\leq\; 2\,\Big(|(\psi, V^{(12)}\,\Lambda_-^{(1)}\,F_0^{(1)}\,\psi)| \;+\; |(\psi, F_0^{(1)}\,\Lambda_-^{(1)}\,V^{(12)}\,\psi)|\Big)$$

$$\leq\; 4\,\|V^{(12)}\,\psi\|\cdot\|\Lambda_-^{(1)}\,F_0^{(1)}\,\psi\| \;\leq\; 4\,\|V^{(12)}\,\psi\|\cdot\|F_0^{(1)}\,\psi\| \tag{II.5.13}$$

since $\Lambda_-^{(1)} = \frac{1}{2}(1-\tilde{D}_0)$ has norm unity.

Thus it remains to show the operator boundedness of $F_0^{(1)}$. Since $F_0^{(1)}$ is a one-particle operator, it suffices to take $\varphi \in \Lambda_+(L_2(\mathbb{R}^3)\times\mathbb{C}^4)$. From (I.1.13) for $F_0^{(1)}$ with (II.3.19),

$$(F_0^{(1)}\varphi)(\mathbf{x}) = -\frac{\gamma}{(2\pi)^{\frac{5}{2}}\cdot 2\pi}\int d\mathbf{q}\frac{1}{q^2}\int d\mathbf{p}' e^{i(\mathbf{q}+\mathbf{p}')\mathbf{x}}\frac{1}{E_{p'}+E_{|\mathbf{q}+\mathbf{p}'|}}$$
$$\cdot\Big(1-\tilde{D}_0^{(1)}(\mathbf{q}+\mathbf{p}')\tilde{D}_0^{(1)}(\mathbf{p}')\Big)\,\hat{\varphi}(\mathbf{p}') \tag{II.5.14}$$

such that

$$\|F_0^{(1)}\,\varphi\|^2 \;=\; \int d\mathbf{x}\;\overline{F_0^{(1)}\varphi(\mathbf{x})}\;F_0^{(1)}\,\varphi(\mathbf{x})$$
$$=\;\frac{\gamma^2}{(2\pi)^4}\int d\mathbf{p}\,d\mathbf{p}'\,d\mathbf{q}\;\overline{\hat{\varphi}(\mathbf{p})}\;\Big(1\;-\;\tilde{D}_0^{(1)}(\mathbf{p})\tilde{D}_0^{(1)}(\mathbf{q}+\mathbf{p})\Big)\;\frac{1}{q^2}\;\frac{1}{E_p+E_{|\mathbf{q}+\mathbf{p}|}} \tag{II.5.15}$$
$$\cdot\;\frac{1}{|\mathbf{q}+\mathbf{p}-\mathbf{p}'|^2}\;\frac{1}{E_{p'}+E_{\mathbf{q}+\mathbf{p}|}}\;\Big(1\;-\;\tilde{D}_0^{(1)}(\mathbf{q}+\mathbf{p})\tilde{D}_0^{(1)}(\mathbf{p}')\Big)\;\hat{\varphi}(\mathbf{p}').$$

Let first $m=0$. Then $E_p = p$ and $\tilde{D}_0^{(1)}(\mathbf{p}) = \boldsymbol{\alpha}\hat{\mathbf{p}}$.

We have from (I.3.11) $\hat{\varphi}(\mathbf{p}) \;=\; U_0'^{-1}\binom{\hat{u}(\mathbf{p})}{0} \;=\; \frac{1}{\sqrt{2}}(1-\beta\tilde{D}_0^{(1)}(\mathbf{p}))\binom{\hat{u}(\mathbf{p})}{0}$ with $u \in L_2(\mathbb{R}^3)\times\mathbb{C}^2$ and therefore

$$\overline{\hat{\varphi}(\mathbf{p})}\;\Big(1\;-\;\tilde{D}_0^{(1)}(\mathbf{p})\tilde{D}_0^{(1)}(\mathbf{q}+\mathbf{p})\Big)\;\Big(1\;-\;\tilde{D}_0^{(1)}(\mathbf{q}+\mathbf{p})\tilde{D}_0^{(1)}(\mathbf{p}')\Big)\;\hat{\varphi}_+(\mathbf{p}')$$
$$=\;\overline{\hat{u}(\mathbf{p})}\;\{1-\boldsymbol{\sigma}(\widehat{\mathbf{q}+\mathbf{p}})\cdot\boldsymbol{\sigma}\hat{\mathbf{p}}'+\boldsymbol{\sigma}\hat{\mathbf{p}}\cdot\boldsymbol{\sigma}\hat{\mathbf{p}}'-\boldsymbol{\sigma}\hat{\mathbf{p}}'\cdot\boldsymbol{\sigma}(\widehat{\mathbf{q}+\mathbf{p}})\}\;\hat{u}(\mathbf{p}'). \tag{II.5.16}$$

With the substitution $\mathbf{q}' := \mathbf{q}+\mathbf{p}$ for $\mathbf{q}$, the kernel of (II.5.15) relating to $\hat{u}$ is given by

$$k_{F_0^{(1)*}F_0^{(1)}}(\mathbf{p},\mathbf{p}') \;=\; \frac{\gamma^2}{(2\pi)^4}\int d\mathbf{q}'\;\frac{1}{|\mathbf{q}'-\mathbf{p}|^2}\;\frac{1}{p+q'}\;\frac{1}{|\mathbf{q}'-\mathbf{p}'|^2}\;\frac{1}{p'+q'}$$
$$\{1-\boldsymbol{\sigma}\hat{\mathbf{q}}'\cdot\boldsymbol{\sigma}\hat{\mathbf{p}}'+\boldsymbol{\sigma}\hat{\mathbf{p}}\cdot\boldsymbol{\sigma}\hat{\mathbf{p}}'-\boldsymbol{\sigma}\hat{\mathbf{p}}\cdot\boldsymbol{\sigma}\hat{\mathbf{q}}'\} \tag{II.5.17}$$

This kernel has the same angular dependence of its integrand as the kernel of the massless second-order term b_2 of the Jansen-Hess operator (see (I.3.23) for $m=0$). Therefore, with a partial wave decomposition of $\hat{u}$, the results of BSS(2002) can be used to obtain

$$\int d\mathbf{p}\,d\mathbf{p}'\;\overline{\hat{u}(\mathbf{p})}\;k_{F_0^{(1)*}F_0^{(1)}}(\mathbf{p},\mathbf{p}')\;\hat{u}(\mathbf{p}') \;=\; \sum_\nu\int_0^\infty dp\int_0^\infty dp'\;\overline{\hat{a}_\nu(p)}\;k^{(\nu)}(p,p')\;\hat{a}_\nu(p')$$

$$k^{(\nu)}(p,p') := \Big(\frac{\gamma}{\pi}\Big)^2\int_0^\infty dq'\frac{1}{p+q'}\;\frac{1}{p'+q'}(q_l(q'/p)-q_{l+2s}(q'/p))(q_l(q'/p')-q_{l+2s}(q'/p')) \tag{II.5.18}$$

with the reduced Legendre functions q_l from Appendix B, and $\nu = \{l, M, s\}$. The Lieb and Yau formula turns (II.5.18) into

$$\|F_0^{(1)}\,\varphi\|^2 \;\leq\; \sum_\nu \int_0^\infty dp\; |\hat{a}_\nu(p)|^2 \cdot \left(\frac{\gamma}{\pi}\right)^2\; I_{ls}(p) \tag{II.5.19}$$

$$I_{ls}(p) \;\leq\; I_0(p) := \int_0^\infty dp' \int_0^\infty dq'\; \frac{1}{q'+p}\; \frac{1}{q'+p'}\; (q_0(q'/p) - q_1(q'/p))$$
$$(q_0(q'/p') - q_1(q'/p')) \cdot \frac{f(p)}{f(p')}$$

where use has been made of the fact that the ground-state configuration $l = 0,\ s = \frac{1}{2}$ provides the largest value of $I_{ls}(p)$ (see Appendix C). The convergence generating function f can be set to unity and the integrals in (II.5.19) are evaluated analytically. For example, with $x := p'/q'$ (for p') and subsequently $y := q'/p$ (for q') one gets from Appendix A

$$I_3(p) := -\int_0^\infty dq'\; \frac{1}{q'+p}\; q_1(q'/p) \cdot \int_0^\infty dp'\; \frac{1}{q'+p'}\; q_0(q'/p') \;=\; -1 \cdot \frac{\pi^2}{4}. \tag{II.5.20}$$

The other three contributions to I_0 are calculated in a similar way, giving

$$I_0(p) \;=\; \left(\frac{\pi^2}{4}\right)^2 \;-\; \frac{\pi^2}{4} \;-\; \frac{\pi^2}{4} \;+\; 1 \;=\; \left(\frac{\pi^2}{4} - 1\right)^2. \tag{II.5.21}$$

Therefore, $\|F_0^{(1)}\,\varphi\|^2 \leq \left(\frac{\pi^2}{4} - 1\right)^2 \cdot \left(\frac{\gamma}{\pi}\right)^2 \|\varphi\|^2$. It is easy to verify with the help of (II.3.4) that (II.5.16) holds also for the states in the negative spectral subspace of $D_0^{(1)}$ (with $\hat{u}$ replaced by $\hat{v}$), such that in this subspace, the norm of $F_0^{(1)}$ is the same. Hence from (II.5.13)

$$|(\psi, C^{(12)}\,\psi)| \;\leq\; \|V^{(12)}\,\psi\| \;\cdot 4\|F_0^{(1)}\| \;\cdot \|\psi\| \;=\; c\,\|V^{(12)}\,\psi\| \cdot \|\psi\| \tag{II.5.22}$$

with $c = 4\left(\frac{\pi^2}{4} - 1\right)\frac{\gamma}{\pi}$ which is < 1 for $\gamma < \frac{\pi}{\pi^2 - 4}$.

For $m \neq 0$, there are two possibilities. One can make the additional estimates $|1 - \tilde{D}_0^{(1)}(\mathbf{p})\tilde{D}_0^{(1)}(\mathbf{q})| \;\leq 2$ and $\frac{1}{E_p + E_q} \;\leq\; \frac{1}{p+q}$ after having applied the Lieb and Yau formula directly to (II.5.15). However, this will increase the bound as shown below. With the substitution $\mathbf{q}' := \mathbf{q} + \mathbf{p}$ for $\mathbf{q}$ one obtains

$$\|F_0^{(1)}\,\varphi\|^2 \;\leq\; \frac{\gamma^2}{(2\pi)^4} \cdot 4 \int d\mathbf{p}\; |\hat{\varphi}(\mathbf{p})|^2\; I_m(p)$$

$$I_m(p) := \int d\mathbf{q}'\; \frac{1}{|\mathbf{q}' - \mathbf{p}|^2}\; \frac{1}{p + q'} \int d\mathbf{p}'\; \frac{1}{|\mathbf{q}' - \mathbf{p}'|^2}\; \frac{1}{p' + q'}\; \frac{f(p)}{f(p')}. \tag{II.5.23}$$

Choosing $f(p) = p$, this leads with Appendix A to

$$I_m(p) \;=\; \int d\mathbf{q}'\; \frac{1}{|\mathbf{q}' - \mathbf{p}|^2}\; \frac{1}{p + q'}\; \frac{2\pi p}{q'} \cdot \frac{\pi^2}{4} \;=\; \left(\frac{\pi^3}{2}\right)^2, \tag{II.5.24}$$

such that $\|F_0^{(1)}\varphi\|^2 \leq \frac{4\gamma^2}{(2\pi)^4} \cdot \left(\frac{\pi^3}{2}\right)^2 \|\varphi\|^2$ and therefore

$$\|F_0^{(1)}\| \;\leq\; \frac{2\gamma}{(2\pi)^2}\; \frac{\pi^3}{2} \;=\; \frac{\gamma\pi}{4}. \tag{II.5.25}$$

Hence, $|(\psi, C^{(12)}\psi)| \leq \gamma\pi\, \|V^{(12)}\psi\|$.

Alternatively, we apply a method put forth by Herbst (1977), which will provide the same bound for $F_0^{(1)}$ as in the $m = 0$ case. Using the behaviour of the kernel of $F_0^{(1)}$ under (unitary) dilations d_θ defined in (I.5.1), extracted from (I.3.26) and (II.3.19),

$$k_{F_{0,m}}(\mathbf{q}/\theta, \mathbf{q}'/\theta) \;=\; -\frac{\gamma}{(2\pi)^2}\,\theta^3\,\frac{1}{|\mathbf{q}-\mathbf{q}'|^2}\;\frac{1}{\sqrt{q'^2+m^2\theta^2}+\sqrt{q^2+m^2\theta^2}}$$

$$\cdot\left(1 \;-\; \frac{\boldsymbol{\alpha}\mathbf{q}+\beta m\theta}{\sqrt{q^2+m^2\theta^2}}\;\frac{\boldsymbol{\alpha}\mathbf{q}'+\beta m\theta}{\sqrt{q'^2+m^2\theta^2}}\right) \;=\; \theta^3\, k_{F_{0,m\cdot\theta}}(\mathbf{q},\mathbf{q}') \tag{II.5.26}$$

where the subscript m (respective $m\cdot\theta$) is introduced to refer explicitly to the mass parameter. From an (I.5.5)-type relation for the dilated kernel, one gets $(d_\theta k_{F_{0,m}} d_\theta^{-1})(\mathbf{q},\mathbf{q}') \;=\; \theta^{-3}k_{F_{0,m}}(\mathbf{q}/\theta,\mathbf{q}'/\theta) \;=\; k_{F_{0,m\cdot\theta}}(\mathbf{q},\mathbf{q}')$, and therefore, from the norm invariance under unitary transformations,

$$\|F_{0,m}\| \;=\; \sup_{\|\varphi\|=1}\,(\varphi, F_{0,m}\varphi) \;=\; \sup_{\|\varphi_\theta\|=1}\,(\varphi_\theta, d_\theta F_{0,m} d_\theta^{-1}\,\varphi_\theta)$$

$$=\; \sup_{\|\varphi_\theta\|=1}\,(\varphi_\theta, F_{0,m\cdot\theta}\varphi_\theta) \;=\; \|F_{0,m\cdot\theta}\|. \tag{II.5.27}$$

Performing the limit $\theta\to 0$, the r.h.s. of (II.5.27) becomes independent of m and therefore we get $\|F_0^{(1)}\| \;\leq \frac{\gamma}{\pi}\,(\frac{\pi^2}{4}-1)$ for all $m\geq 0$. ∎

Proof of (ii).
We will show that

$$(\psi, V^{(12)}\,\psi) \;+\; (\psi, C^{(12)}\,\psi) \;\geq\; (\psi, V^{(12)}\,\psi) \;-\; |(\psi, C^{(12)}\,\psi)|$$

$$\geq\; (1 \;-\; C\pi\gamma)\;(\psi, V^{(12)}\,\psi) \tag{II.5.28}$$

from which (ii) is an immediate consequence. Since $V^{(12)}$ is diagonal in coordinate space, we use the same strategy as for the proof of Proposition I.3 in the massive case, and transform the kernel of $C^{(12)}$ into coordinate space. With the help of the inverse Fourier transform of (II.3.5) we obtain from (II.4.8)

$$(\psi, C^{(12)}\,\psi) \;=\; \frac{1}{(2\pi)^6}\int d\mathbf{x}_1\,d\mathbf{x}_2\;\overline{\psi(\mathbf{x}_1,\mathbf{x}_2)}\int d\mathbf{x}_1'\,d\mathbf{x}_2'\;k(\mathbf{x}_1,\mathbf{x}_2;\mathbf{x}_1',\mathbf{x}_2')\;\psi(\mathbf{x}_1',\mathbf{x}_2') \tag{II.5.29}$$

$$k(\mathbf{x}_1,\mathbf{x}_2;\mathbf{x}_1',\mathbf{x}_2') := \int d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_1' d\mathbf{p}_2'\, e^{i\mathbf{p}_1\mathbf{x}_1}e^{i\mathbf{p}_2\mathbf{x}_2}k_{C^{(12)}}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2')e^{-i\mathbf{p}_1'\mathbf{x}_1'}e^{-i\mathbf{p}_2'\mathbf{x}_2'}$$

with the kernel $k_{C^{(12)}}$ defined in (II.4.10). Then we use the generalised Lieb and Yau formula, Lemma II.1, to estimate

$$(\psi, V^{(12)}\,\psi) \;-\; |(\psi, C^{(12)}\,\psi)| \;\geq\; \int d\mathbf{x}_1\,d\mathbf{x}_2\;|\psi(\mathbf{x}_1,\mathbf{x}_2)|^2\;\left\{\frac{e^2}{|\mathbf{x}_1-\mathbf{x}_2|}\right.$$

$$\left.-\;\frac{1}{(2\pi)^6}\int d\mathbf{x}_1'\,d\mathbf{x}_2'\;\;|k(\mathbf{x}_1,\mathbf{x}_2;\mathbf{x}_1',\mathbf{x}_2')|\;\frac{f(x_1)}{f(x_1')}\cdot\frac{g(x_2)}{g(x_2')}\right\}. \tag{II.5.30}$$

In Appendix F the second integral is estimated, with the result

$$(\psi, V^{(12)}\,\psi) \;-\; |(\psi, C^{(12)}\,\psi)| \;\geq\; \int d\mathbf{x}_1\,d\mathbf{x}_2\;|\psi(\mathbf{x}_1,\mathbf{x}_2)|^2\;\left\{\frac{e^2}{|\mathbf{x}_1-\mathbf{x}_2|}\;-\;\frac{C\pi\gamma e^2}{|\mathbf{x}_1-\mathbf{x}_2|}\right\} \tag{II.5.31}$$

which proves (II.5.28). ∎

Lemma II.5 (Translation property)**.**
Let T_a defined on $\mathcal{H}_{+,2}$ be the translation $T_a\psi(\mathbf{x}_1,\mathbf{x}_2) \;=\; \psi(\mathbf{x}_1+\mathbf{a},\mathbf{x}_2+\mathbf{a})$ $=: \psi_a(\mathbf{x}_1,\mathbf{x}_2)$. Then for $\psi\in\mathcal{H}_{+,2}$,

$$\lim_{a\to\infty}\,(\psi_a, (V^{(12)} \;+\; C^{(12)})\;\psi_a) \;=\; (\psi, V^{(12)}\;\psi). \tag{II.5.32}$$

An immediate consequence is $\lim\limits_{a\to\infty} \|(V^{(12)} + C^{(12)})\,\psi_a\| \;=\; \|V^{(12)}\psi\|.$

Proof. Upon using the substitution $\mathbf{x}_i := \mathbf{y}_i + \mathbf{a},\;\; i = 1,2,$ one gets

$$(T_a\psi, V^{(12)}\,T_a\psi) \;=\; (\psi_a, V^{(12)}\,\psi_a)$$

$$= \int d\mathbf{y}_1\,d\mathbf{y}_2\,\overline{\psi(\mathbf{y}_1+\mathbf{a},\mathbf{y}_2+\mathbf{a})}\;\frac{e^2}{|\mathbf{y}_1-\mathbf{y}_2|}\;\psi(\mathbf{y}_1+\mathbf{a},\mathbf{y}_2+\mathbf{a})$$

$$= \int d\mathbf{x}_1\;d\mathbf{x}_2\;\overline{\psi(\mathbf{x}_1,\mathbf{x}_2)}\;\frac{e^2}{|x_1-x_2|}\;\psi(\mathbf{x}_1,\mathbf{x}_2) \;=\; (\psi, V^{(12)}\,\psi) \tag{II.5.33}$$

which means that $V^{(12)}$ is translational invariant. With $C_1^{(12)} = V^{(12)}\Lambda_-^{(1)}F_0^{(1)} + F_0^{(1)}\Lambda_-^{(1)}V^{(12)}$ we continue by showing that $\Lambda_-^{(1)}$ is T_a-invariant as well, while $T_a^* F_0^{(1)} T_a$ vanishes for $a\to\infty$. From this and from the unitarity relation $T_a^*T_a = 1$ one gets the desired result,

$$\lim_{a\to\infty}(\psi_a, C^{(12)}\,\psi_a) \;=\; 2\lim_{a\to\infty}(\psi_a, C_1^{(12)}\,\psi_a) \;=\; 0. \tag{II.5.34}$$

We start by showing that $\tilde{D}_0^{(1)}$ is T_a-invariant. From comparison with (II.5.33),

$$T_a^*\tilde{D}_0^{(1)}T_a \;=\; T_a^*\left(\frac{-i\sum_{k=1}^3 \alpha_k\partial_{x_{1k}} + \beta m}{\sqrt{-\sum_{k=1}^3 \partial^2_{x_{1k}} + m^2}}\right)T_a \tag{II.5.35}$$

$$= \frac{-i\sum_{k=1}^3 \alpha_k\partial_{(x_{1k}-a_k)} + \beta m}{\sqrt{-\sum_{k=1}^3(\partial_{x_{1k}-a_k}) + m^2}} \;=\; \tilde{D}_0^{(1)}$$

where $\partial_{x_{1k}} := \partial/\partial x_{1k}$ with x_{1k} the k-th component of $\mathbf{x}_1$. As a consequence, $\Lambda_1^{(1)} = \frac{1}{2}(1-\tilde{D}_0^{(1)})$ is T_a-invariant, as well as $D_0^{(1)}$.

Using the representation (II.2.9) for $F_0^{(1)}$, one gets further

$$T_a^*F_0^{(1)}T_a \;=\; -\frac{\gamma}{2\pi}\int_{-\infty}^{\infty}d\eta\left(T_a^*\;\frac{1}{D_0^{(1)}+i\eta}\;T_a\right)\left(T_a^*\;\frac{1}{x_1}\;T_a\right)\left(T_a^*\;\frac{1}{D_0^{(1)}+i\eta}\;T_a\right)$$

$$= -\frac{\gamma}{2\pi}\int_{-\infty}^{\infty}d\eta\;\frac{1}{D_0^{(1)}+i\eta}\;\frac{1}{|\mathbf{x}_1-\mathbf{a}|}\;\frac{1}{D_0^{(1)}+i\eta} \;\longrightarrow\; 0 \qquad (a\to\infty). \tag{II.5.36}$$

■

An important application of this result will concern the spectrum of the transformed Coulomb-Dirac operator (see section II.6).

c) Estimate of $V^{(12)}$

In order to prove subordinacy of the summed interaction terms for a largest possible critical potential strength, an improved estimate of the Coulomb field $V^{(12)}$ is needed. For $\psi\in\mathcal{A}(H_{1/2}(\mathbb{R}^3)\times\mathbb{C}^4)^2$, Kato's inequality provides the sharp form bound $(\psi, V^{(12)}\psi) \;\le\; \frac{\pi}{4}e^2\,(\psi,(p_1+p_2)\psi)$ (BBHS 1999). However, if in addition ψ is in the positive spectral subspace of the free Dirac operator, the form bound turns out to be smaller.

To this aim we first consider the one-particle case.

Lemma II.6 (Improved estimate of Coulomb field)**.**
Let $\varphi\in\mathcal{H}_{+,1}$ be a one-particle function in the positive spectral subspace of the free Dirac operator. Then

$$(\varphi, \frac{1}{x}\,\varphi) \;\le\; \frac{1}{\gamma_{BR}}\,(\varphi, E_p\,\varphi) \tag{II.5.37}$$

where $\gamma_{BR} = \frac{2}{\pi/2 + 2/\pi} = 0.906$ *is the critical potential strength for stability of the Brown-Ravenhall operator.*

This bound holds also for $\varphi \in \Lambda_-(H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4)$ (DES 2000).

Proof. For the massless case we use an inequality derived by BSS (2003) in the course of their proof of positivity of the massless Brown-Ravenhall operator (their Theorem 2). With the equivalence of expectation values (Theorem I.2) for $u \in H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2$ and $\varphi \in \Lambda_+(H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4)$, one has

$$(\varphi, (D_0 - \frac{\gamma}{x})\, \varphi) = (\begin{pmatrix} u \\ 0 \end{pmatrix}, U_0\, (D_0 - \frac{\gamma}{x})\, U_0^{-1} \begin{pmatrix} u \\ 0 \end{pmatrix}) = (u, (b_0 + b_1)\, u)$$

$$\geq (u, p\, u)\, (1 - \frac{\gamma}{\gamma_{BR}}). \tag{II.5.38}$$

Since φ is an eigenstate of D_0 with $D_0 \varphi = p\, \varphi$ (for $m = 0$), and $(u, p\, u) = (\varphi, p\, \varphi)$ because the zero-order Foldy-Wouthuysen transformation U_0 commutes with p, this leads to

$$(\varphi, p\, \varphi) - \gamma\, (\varphi, \frac{1}{x}\, \varphi) \geq (\varphi, p\, \varphi) - \frac{\gamma}{\gamma_{BR}}\, (\varphi, p\, \varphi) \tag{II.5.39}$$

which proves the lemma since $E_p(m = 0) = p$.

Based on the work of Tix (1998), Burenkov and Evans (1998) have derived for the case $m \neq 0$ an inequality corresponding to (II.5.38),

$$(\varphi, (D_0 - \frac{\gamma}{x})\, \varphi) \geq (1 - \frac{\gamma}{\gamma_{BR}})\, (\varphi, E_p\, \varphi), \tag{II.5.40}$$

from which the assertion (II.5.37) follows in the same way as for $m = 0$. ∎

Now we turn to the electron-electron potential.

Lemma II.7 ($|T|$-form boundedness of $V^{(12)}$**).**
Let $\psi \in \mathcal{H}_{+,2}$ *and* $T = D_0^{(1)} + D_0^{(2)}$. *Then one has the estimate*

$$(\psi, V^{(12)}\, \psi) \leq \frac{e^2}{2\gamma_{BR}}\, (\psi, (E_{p_1} + E_{p_2})\, \psi) \tag{II.5.41}$$

with form bound $e^2/(2\gamma_{BR}) = 0.004$.

Proof. Following Bach et al (BBHS 1999) we get with the substitution $\mathbf{y}_1 := \mathbf{x}_1 - \mathbf{x}_2$ for $\mathbf{x}_1$,

$$(\psi, V^{(12)}\, \psi) = \int d\mathbf{x}_1\, d\mathbf{x}_2\, \overline{\psi(\mathbf{x}_1, \mathbf{x}_2)}\, \frac{e^2}{|\mathbf{x}_1 - \mathbf{x}_2|}\, \psi(\mathbf{x}_1, \mathbf{x}_2)$$

$$= e^2 \int d\mathbf{x}_2 \int d\mathbf{y}_1\, \overline{\varphi_{x_2}(\mathbf{y}_1)}\, \frac{1}{y_1}\, \varphi_{x_2}(\mathbf{y}_1) \tag{II.5.42}$$

where $\varphi_{x_2}(\mathbf{y}_1) := \psi(\mathbf{y}_1 + \mathbf{x}_2, \mathbf{x}_2)$. Introducing the Fourier transform $\hat{\varphi}_{x_2}(\mathbf{p}_1)$ of $\varphi_{x_2}(\mathbf{y}_1)$ with respect to $\mathbf{y}_1$ and using Lemma II.6,

$$(\psi, V^{(12)}\, \psi) \leq \frac{e^2}{\gamma_{BR}} \int d\mathbf{x}_2\, (\hat{\varphi}_{x_2}(\mathbf{p}_1), E_{p_1}\, \hat{\varphi}_{x_2}(\mathbf{p}_1)) \tag{II.5.43}$$

$$= \frac{e^2}{\gamma_{BR}} \int d\mathbf{x}_2\, (\varphi_{x_2}(\mathbf{y}_1), \sqrt{-\Delta_{y_1} + m^2}\, \varphi_{x_2}(\mathbf{y}_1)) = \frac{e^2}{\gamma_{BR}}\, (\psi, E_{p_1}\, \psi)$$

$$= \frac{e^2}{2\gamma_{BR}}\, (\psi, (E_{p_1} + E_{p_2})\, \psi).$$

where in the second line, $\mathbf{x}_1 = \mathbf{y}_1 + \mathbf{x}_2$ was substituted back, $E_{p_1} = \sqrt{-\Delta_{x_1} + m^2}$ and the symmetry property of ψ were used. ∎

d) $|T|$-form boundedness of the perturbation and positivity

We start by collecting some results for the (one-particle) Jansen-Hess operator from section I, which will be needed below.

Lemma II.8 (Form bounds for one-particle operators).

Let $D_0^{(k)} + V^{(k)} + \frac{i}{2}\,[W_1^{(k)}, B_1^{(k)}]$ be the single-particle operator up to second order as defined in section I. Then for $\psi \in \mathcal{H}_{+,2}$, the following inequalities hold

(i) *massless case, $m = 0$:*

$$V^{(k)} \;+\; \frac{i}{2}\,[W_1^{(k)}, B_1^{(k)}] \;\leq\; 0 \qquad \textit{for}\; \gamma \;\leq\; 4/\pi \tag{II.5.44}$$

$$\frac{i}{2}\,[W_1^{(k)}, B_1^{(k)}] \;\geq\; 0 \tag{II.5.45}$$

$$(\psi, (D_0^{(k)} + V^{(k)} + \frac{i}{2}\,[W_1^{(k)}, B_1^{(k)}]\,)\,\psi) \;\geq\; (1 - \frac{\gamma}{\gamma_{BR}} \;+ d\gamma^2)\,(\psi, D_0^{(k)}\,\psi) \tag{II.5.46}$$

with $d = \frac{1}{8}\,(\pi/2\, - 2/\pi)^2$.

(ii) *massive case, $m \neq 0$:*

$$(\psi, \frac{i}{2}\,[W_1^{(k)}, B_1^{(k)}]\;\psi) \;\geq\; -md_0\gamma^2\;(\psi, \psi) \tag{II.5.47}$$

with $d_0 := 8 + 12\sqrt{2}$,

$$(\psi, (D_0^{(k)} + V^{(k)} + \frac{i}{2}\,[W_1^{(k)}, B_1^{(k)}]\,)\,\psi) \;\geq\; (1 - \frac{\gamma}{\gamma_{BR}} \;- d\gamma^2)\,(\psi, D_0^{(k)}\,\psi) \tag{II.5.48}$$

$$(\psi, (V^{(k)} \;+\; \frac{i}{2}\,[W_1^{(k)}, B_1^{(k)}]\,)\;\psi) \;\leq\; m\;(d_0\gamma^2 \;+\; \frac{3}{2}\gamma)\;(\psi, \psi) \qquad \textit{for}\; \gamma \leq 4/\pi. \tag{II.5.49}$$

Proof. If an inequality holds in the single-particle case, one can easily show its validity in the case of two-particle expectation values. Let us start with (II.5.44). We have to prove that (for particle 1)

$$(\psi, (V^{(1)} \;+\; \frac{i}{2}\,[W_1^{(1)}, B_1^{(1)}]\,)\;\psi) \;\leq\; 0. \tag{II.5.50}$$

From Proposition I.3 we know that for $m = 0$ and $\gamma \leq 4/\pi$,

$$(u, (b_1^{(1)} \;+\; b_2^{(1)})\;u) \;\leq\; 0 \qquad \forall\, u \in H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^2. \tag{II.5.51}$$

Using the equivalence with the Sobolev transformation, we derive for $\varphi = U_0^{-1}\,\binom{u}{0}$ $\in \Lambda_+(H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4)$,

$$(\varphi, (V^{(1)} \;+\; \frac{i}{2}\,[W_1^{(1)}, B_1^{(1)}]\,)\,\varphi) \;\leq\; 0. \tag{II.5.52}$$

Let $\psi = \psi(\mathbf{x}_1, \mathbf{x}_2) \in \mathcal{H}_{+,2}$ and set $\psi(\mathbf{x}_1, \mathbf{x}_2) =: \psi_{x_2}(\mathbf{x}_1)$. Then $\Lambda_+^{(1)}\,\psi_{x_2}(\mathbf{x}_1) = \psi_{x_2}(\mathbf{x}_1)$, i.e. for fixed $\mathbf{x}_2$, $\psi_{x_2}(\mathbf{x}_1) \in \Lambda_+^{(1)}(H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4)$, such that (II.5.52) holds,

$$(\psi_{x_2}, (V^{(1)} \;+\; \frac{i}{2}\,[W_1^{(1)}, B_1^{(1)}]\,)\;\psi_{x_2}) \;\leq\; 0. \tag{II.5.53}$$

Integration over $\mathbf{x}_2$ yields the desired result (II.5.50).

The inequalities (II.5.45) and (II.5.46) are derived in a similar way from $(u, b_2\,u)$ ≥ 0 and from $(u, b\,u) \;\geq (1\, - \gamma/\gamma_{BR}\, + d\gamma^2)(u, p\,u)$ (BSS 2002, see also Lemma I.9).

From the boundedness of the difference between massive and massless second-order term (BSS 2002, see also Lemma I.10),

$$-md_0\gamma^2\;(u, u) \;\leq\; (u, (b_{2m} \;-\; b_2)\;u) \;\leq\; md_0\gamma^2\;(u, u) \tag{II.5.54}$$

one has $(u, b_{2m}\, u) \geq (u, b_2\, u) - md_0\gamma^2\,(u,u) \geq -md_0\gamma^2\,(u,u),$ and hence (II.5.47) holds. Inequality (II.5.48) results from $(u, b_m u) \geq (1 - \gamma/\gamma_{BR} - d\gamma^2)(u, E_p\, u)$ (Proposition I.5), whereas the last inequality (II.5.49) is based on (II.5.54) and Lemma I.8,

$$(u, (b_{1m} - b_1)\, u) \;\leq\; \frac{3}{2}\, m\gamma\, (u,u), \tag{II.5.55}$$

such that

$$(u, (b_{1m} + b_{2m})\, u) \;\leq\; (u, (b_1 + b_2)\, u) \;+\; (md_0\gamma^2 + \frac{3}{2}\, m\gamma)\,(u,u)$$

$$\leq\; m\,(d_0\gamma^2 + \frac{3}{2}\,\gamma)\,(u,u) \tag{II.5.56}$$

where (II.5.51) was used. ■

Proposition II.3 (|T|-form boundedness and positivity)**.**
Let $H^{(2)}$ be the transformed Coulomb-Dirac operator up to second order in the coupling constant e^2, and let $\psi \in \mathcal{H}_{+,2}$ be an antisymmetrised two-particle spinor. Within this space, one has

$$(\psi, H^{(2)}\,\psi) \;=\; (\psi, \left(\sum_{k=1}^{2}(D_0^{(k)} + V^{(k)} + \frac{i}{2}\,[W_1^{(k)}, B_1^{(k)}]\,) + V^{(12)} + 2C_1^{(12)}\right)\psi)$$

$$=: (\psi, (T + W)\,\psi) \tag{II.5.57}$$

with $C_1^{(12)}$ from Lemma II.4 and $T := D_0^{(1)} + D_0^{(2)}$. The total potential W is $|T|$-form bounded,

$$|(\psi, W\,\psi)| \;\leq\; c\,(\psi, T\,\psi) \;+\; C\,(\psi,\psi) \tag{II.5.58}$$

with form bound $c < 1$ for $\gamma < 0.986$ $(Z \leq 135)$ and $C = 0$ if $m = 0$, and $c < 1$ for $\gamma < 0.89$ $(Z \leq 122)$ if $m \neq 0$. We also have positivity,

$$(\psi, (T + W)\,\psi) \;\geq\; 0, \tag{II.5.59}$$

for $\gamma < 0.986$ if $m = 0$, and for $\gamma < 0.825$ $(Z \leq 113)$ if $m \neq 0$.

Proof. We consider first the massless case and estimate W from above. With (II.5.44) and Lemmata II.4 and II.7,

$$(\psi, W\psi) \leq (\psi, (V^{(12)} + 2C_1^{(12)})\psi) \leq \frac{e^2}{2\gamma_{BR}}(\psi, (p_1 + p_2)\psi) + \gamma e^2 \frac{\pi^2}{4}(\psi, (p_1 + p_2)\psi)$$

$$= \; c_h\,(\psi, T\,\psi) \qquad \text{with } \; c_h := \frac{e^2}{2\gamma_{BR}} \;+\; \frac{\gamma e^2 \pi^2}{4}. \tag{II.5.60}$$

One has $c_h < e^2$ for $\gamma < 0.18$ and $c_h < 1$ for $\gamma < 55.3$.

For the estimate of W from below, we use the result of BBS (2002), inequality (II.5.46). Then with $V^{(12)} \geq 0$ and Lemma II.4,

$$(\psi, W\,\psi) \;\geq\; (-\frac{\gamma}{\gamma_{BR}} + d\gamma^2)\,(\psi, T\,\psi) \;-\; \gamma e^2\,\frac{\pi^2}{4}\,(\psi, T\,\psi) \;=\; -c_l\,(\psi, T\,\psi), \tag{II.5.61}$$

with $c_l := \gamma\,(\frac{1}{\gamma_{BR}} + e^2\pi^2/4) - d\gamma^2$.

We have $c_l < 1$ for $\gamma < 0.986$. Therefore, W is $|T|$-form bounded,

$$|(\psi, W\,\psi)| \;\leq\; c\,(\psi, T\,\psi) \qquad \text{with } \; c := \max\{c_h, c_l\}. \tag{II.5.62}$$

$c = c_l$ for $0.004 < \gamma < 10.1$. For $\gamma \leq 0.004$, one has $c = c_h \ll 1$.

Positivity of the transformed operator follows immediately from (II.5.61),

$$(\psi, (T + W)\,\psi) \;\geq\; (1 - c_l)\,(\psi, T\,\psi) \;>\; 0 \text{ for } c_l < 1. \tag{II.5.63}$$

Now we turn to the case $m \neq 0$. First we estimate W from above, using (II.5.49) as well as the second inequality of (II.5.60) which also holds for $m \neq 0$:

$$(\psi, W\,\psi) \;\leq\; 2m\,(d_0\gamma^2 \,+\, \frac{3}{2}\gamma)\,(\psi,\psi) \;+\; c_h\,(\psi,(E_{p_1}+E_{p_2})\,\psi). \tag{II.5.64}$$

For the estimate of W from below, the proof of Lemma II.7 shows that $(\psi, \frac{1}{x_1}\,\psi) \leq \frac{1}{\gamma_{BR}}\,(\psi, p_1\,\psi)$. Hence, for $V^{(1)} = -\gamma/x_1$,

$$(\psi, V^{(1)}\,\psi) \;\geq\; -\frac{\gamma}{\gamma_{BR}}\,(\psi, p_1\,\psi) \;\geq\; -\frac{\gamma}{\gamma_{BR}}\,(\psi, E_{p_1}\,\psi). \tag{II.5.65}$$

Then, with (II.5.47), $V^{(12)} \geq 0$ and (II.5.2):

$$(\psi, W\,\psi) \;\geq\; -\frac{\gamma}{\gamma_{BR}}\,(\psi,(E_{p_1}+E_{p_2})\,\psi) - 2md_0\gamma^2\,(\psi,\psi) - \gamma e^2\,\frac{\pi^2}{4}\,(\psi,(E_{p_1}+E_{p_2})\,\psi)$$

$$= \; -\tilde{c}_l\,(\psi, T\,\psi) \;-\; 2md_0\gamma^2\,(\psi,\psi), \tag{II.5.66}$$

with $\tilde{c}_l := \gamma(\frac{1}{\gamma_{BR}} + e^2\pi^2/4)$ which is < 1 for $\gamma < 0.89$.

As a consequence, $|T|$-form boundedness of W is expressed in the following way

$$|(\psi, W\,\psi)| \;\leq\; c\,(\psi, T\,\psi) \;+\; 2m\,(d_0\gamma^2 \,+\, \frac{3}{2}\gamma)\,(\psi,\psi) \tag{II.5.67}$$

where

$$c := \;\max\,\{c_h, \tilde{c}_l\} \tag{II.5.68}$$

and $c = \tilde{c}_l$ for $\gamma > e^2/2$.

In order to establish positivity, the single-particle estimates are used. With (II.5.48), one finds

$$(\psi,(T+W)\,\psi) \;\geq\; (1 \,-\, \frac{\gamma}{\gamma_{BR}} \,-\, d\gamma^2)\,(\psi, T\,\psi) \;-\; \gamma e^2\,\frac{\pi^2}{4}\,(\psi, T\,\psi)$$

$$= \; c_0\,(\psi, T\,\psi) \qquad \text{with } \; c_0 := 1 \,-\, \gamma\,(\frac{1}{\gamma_{BR}} \,+\, e^2\,\frac{\pi^2}{4}) \;-\; d\gamma^2. \tag{II.5.69}$$

Positivity is obtained for $c_0 > 0$, i.e. $\gamma < 0.825$. ∎

We note that due to the smallness of e^2 (with respect to γ) for high nuclear charges, the critical potential strength for positivity of the two-particle operator is close to those for positivity of the Jansen-Hess operator.

Collecting results, the $|T|$-form boundedness of the total potential W with form bound < 1 ensures that $T + W$ is well defined as a form sum of T and W with the form domain of T. Moreover, the semiboundedness of the transformed Coulomb-Dirac operator allows for its Friedrichs extension to a self-adjoint operator on the Hilbert space $(\Lambda_+^{(1)} \otimes \Lambda_+^{(2)})(\mathcal{A}(L_2(\mathbb{R}^3) \times \mathbb{C}^4)^2)$.

II.6. **The spectrum of the transformed Coulomb-Dirac operator.**

In this section it is shown that the free-particle positive spectrum is a subset of the essential spectrum of the transformed Coulomb-Dirac operator $H^{(2)}$ and that the second-order two-particle interaction does not change the essential spectrum of $H^{(2)}$. Moreover we will prove that in the massless case, there are no eigenvalues embedded in the essential spectrum. Let us start with some known results.

We recall that we are only interested in expectation values (and the resulting spectrum) of $H^{(2)}$ taken with states ψ in the positive spectral subspace $\mathcal{H}_{+,2}$ of the free two-particle operator $T = D_0^{(1)} + D_0^{(2)}$. With this restriction, one has $\sigma(T) = \sigma_{ess}(T) = [2m, \infty)$. This is easily seen from

$$(\widehat{T\psi})(\mathbf{p}_1, \mathbf{p}_2) \;=\; (E_{p_1} \,+\, E_{p_2})\, \hat{\psi}(\mathbf{p}_1, \mathbf{p}_2) \;=\; (\sqrt{p_1^2 + m^2} \,+\, \sqrt{p_2^2 + m^2}\,)\, \hat{\psi}(\mathbf{p}_1, \mathbf{p}_2). \tag{II.6.1}$$

With $H^{(2)}$ from (II.5.57) we define the abbreviations

$$H^{(2)} \;=\; T + W, \qquad W \;=\; W^{(1)} \,+\, W^{(2)} \,+\, V^{(12)} \,+\, 2C_1^{(12)}, \tag{II.6.2}$$

with $W^{(k)} := V^{(k)} + \frac{i}{2}\,[W_1^{(k)}, B_1^{(k)}],\;\; k = 1,2$ the potential term of the Jansen-Hess operator for particle k.

Let $\sigma(D_0^{(k)} + W^{(k)})$ be the respective one-particle spectrum. Dropping for a moment all two-particle interactions, the spectrum of the sum of the single-particle operators is given by (Reed-Simon 1980, Corollary to Theorem VIII.33)

$$\sigma(T + W^{(1)} + W^{(2)}) \;=\; \overline{\{\lambda_1 + \lambda_2 :\; \lambda_k \in \sigma(D_0^{(k)} + W^{(k)}),\; k = 1,2\}}. \tag{II.6.3}$$

So if $D_0^{(1)} + W^{(1)}$ has a bound ground state with eigenvalue $0 < \lambda_{01} < m$, then the essential spectrum of $T + W^{(1)} + W^{(2)}$ starts at $\lambda_{01} + m$, i.e.

$$\sigma_{ess}(T + W^{(1)} + W^{(2)}) \;=\; [m + \inf_{\lambda_1 \in \sigma(D_0^{(1)} + W^{(1)})} \lambda_1, \infty) \tag{II.6.4}$$

(Reed-Simon 1978, p.121). This is true because for the Jansen-Hess operator $D_0^{(1)} + W^{(1)}$, the essential spectrum is the same as for $D_0^{(1)}$ for subcritical potential strength, namely $[m, \infty)$ (see Theorem I.3).

Let us now switch on the two-particle interactions. We aim at proving the following properties of the spectrum.

Theorem II.1 (Location of essential spectrum)**.**
Let $H^{(2)} = T + W$ with $T = D_0^{(1)} + D_0^{(2)}$ and $W = \sum_{k=1}^{2} W^{(k)} + V^{(12)} + 2C_1^{(12)}$ be the transformed Coulomb-Dirac operator up to second order in the coupling constant e^2, acting on $\mathcal{H}_{+,2}^1 := (\Lambda_+^{(1)} \otimes \Lambda_+^{(2)})(\mathcal{A}(H_1(\mathbb{R}^3) \times \mathbb{C}^4)^2)$. Then for potential strengths $\gamma < 0.89$, the spectrum has the following properties

(i)

$$[2m, \infty) \;=\; \sigma(T) \;\subset\; \sigma(T + V^{(12)}) \;\subset \sigma(H^{(2)}) \tag{II.6.5}$$

(ii)

$$[2m, \infty) \;=\; \sigma_{ess}(T) \;\subset\; \sigma_{ess}(T + V^{(12)}) \;\subset \sigma_{ess}(H^{(2)}) \tag{II.6.6}$$

and for $\gamma < 0.654$,

(iii)

$$\sigma_{ess}(H^{(2)}) \;=\; \sigma_{ess}(T \,+\, \sum_{k=1}^{2} W^{(k)} \,+\, V^{(12)}). \tag{II.6.7}$$

The bound 0.89 on γ arises from the requirement that $H^{(2)}$ is well-defined (see Proposition II.3).
For the proof of inclusions (i) and (ii) we use the behaviour under translations (Hunziger 1966, Reed-Simon 1978, p.370, problem 45), together with the Weyl criterion (Weidmann 1980, Theorem 7.22).

Lemma II.9 (Weyl criterion)**.**
Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$. Then $\lambda \in \sigma(A)$ iff there exists a sequence $(\psi_l)_{l\in\mathbb{N}}$ in the domain of A with $\|\psi_l\| > 0$ such that

$$\|(A \,-\, \lambda)\, \psi_l\| \;\longrightarrow\; 0 \qquad (l \to \infty). \tag{II.6.8}$$

If $(\psi_l)_{l\in\mathbb{N}}$ can be chosen orthogonal then $\lambda \in \sigma_{ess}(A)$.

In the following, all symmetric operators are considered as self-adjoint by means of their Friedrichs extension (which exists for subcritical γ).

Proof of (i) and (ii).
Let T_a be the translation defined in Lemma II.5 and let $a := n \in \mathbb{N}$. Then $(T_n)_{n\in\mathbb{N}}$ induces a sequence $(\psi_n)_{n\in\mathbb{N}}$ where $a \to \infty$ corresponds to $n \to \infty$.

From the proof of Lemma II.5 we know that $D_0^{(k)}$ and $V^{(12)}$ are T_n-invariant, while $(\psi_n, W^{(k)}\psi_n)$ and $(\psi_n, C_1^{(12)}\psi_n)$ tend to zero when $n \to \infty$. Hence

$$\lim_{n\to\infty} \|(H^{(2)} - \lambda)\,\psi_n\|^2 \;=\; \lim_{n\to\infty} (\psi_n,\, (H^{(2)} - \lambda)^2\,\psi_n) \;=\; (\psi,\, (T + V^{(12)} - \lambda)^2\,\psi)$$

$$=\; \|(T + V^{(12)} - \lambda)\,\psi\|^2. \tag{II.6.9}$$

Now let $\lambda \in \sigma(T + V^{(12)})$. Then there exists a sequence $(\psi_l)_{l\in\mathbb{N}}$ such that $\|(T + V^{(12)} - \lambda)\,\psi_l\| \to 0$ as $l \to \infty$. We identify the ψ from (II.6.9) with ψ_l and translate each ψ_l with T_n. Constructing a diagonal subsequence $(\psi_{l,l})_{l\in\mathbb{N}}$ of the sequence $(\psi_{l,n})_{n,l\in\mathbb{N}}$ we get

$$\lim_{l\to\infty} \|(H^{(2)} - \lambda)\,\psi_{l,l}\|^2 \;=\; \lim_{l\to\infty} \|(T + V^{(12)} - \lambda)\,\psi_l\|^2 \;=\; 0 \tag{II.6.10}$$

such that $\lambda \in \sigma(H^{(2)})$. This proves $\sigma(T + V^{(12)}) \subset \sigma(H^{(2)})$.

In order to prove the first inclusion of (i), we choose a translation $T_b^{(1)}$ which affects only the coordinate $\mathbf{x}_1$, i.e. $T_b^{(1)}\psi(\mathbf{x}_1, \mathbf{x}_2) = \psi(\mathbf{x}_1 + \mathbf{b}, \mathbf{x}_2) =: \psi_b^{(1)}(\mathbf{x}_1, \mathbf{x}_2)$. This translation leaves T invariant, but not $V^{(12)}$, since
$T_b^{(1)*}\,V^{(12)}\,T_b^{(1)} \;=\; \dfrac{e^2}{|\mathbf{x}_1 - \mathbf{b} - \mathbf{x}_2|} \;\to 0$ as $b \to \infty$. As a consequence,

$$\lim_{b\to\infty} \|(T + V^{(12)} - \lambda)\,\psi_b^{(1)}\|^2 \;=\; \|(T - \lambda)\,\psi\|^2. \tag{II.6.11}$$

We set $b := n$ to define a sequence $(\psi_n^{(1)})_{n\in\mathbb{N}}$ and use the same argumentation to prove that for $\lambda \in \sigma(T)$, we have $\lambda \in \sigma(T + V^{(12)})$.

In order to prove (ii), we take the sequence $(\psi_l)_{l\in\mathbb{N}}$ to be an orthogonal sequence and construct via translation with T_n the diagonal subsequence $(\psi_{l,l})_{l\in\mathbb{N}}$. Since the $(\psi_l)_{l\in\mathbb{N}}$ are orthogonal, the translated functions $(\psi_{l,l})_{l\in\mathbb{N}}$ are linearly independent and can be orthogonalised. Hence for $\lambda \in \sigma_{ess}(T + V^{(12)})$, we have $\lambda \in \sigma_{ess}(H^{(2)})$. By choosing the sequence $(\psi_n^{(1)})_{n\in\mathbb{N}}$ orthogonal, it follows in a similar way that $\sigma_{ess}(T) \subset \sigma_{ess}(T + V^{(12)})$.

We remark that this proof holds both for $m = 0$ and $m \neq 0$. ∎

Proof of (iii).
For the proof of equality (II.6.7) it is sufficient to show that the resolvent difference

$$R_\mu := \; (H^{(2)} + \mu)^{-1} \;-\; (H_v + \mu)^{-1}, \tag{II.6.12}$$

$$H_v := \; T \,+\, \sum_{k=1}^{2} W^{(k)} \,+\, V^{(12)}$$

is compact for a suitable $\mu \geq 1$ (see section I.5). Using the second resolvent identity, we decompose

$$R_\mu \;=\; -\,(H_v + \mu)^{-1}\, 2C_1^{(12)}\, (H^{(2)} + \mu)^{-1} \tag{II.6.13}$$

$$=\; -\,\left[(H_v + \mu)^{-1}\,(T + \mu)\right] \cdot \left\{(T + \mu)^{-1}\, 2C_1^{(12)}\, (T + \mu)^{-1}\right\} \cdot \left[(T + \mu)\,(H^{(2)} + \mu)^{-1}\right]$$

and show that the operator in curly brackets is compact and the adjacent two factors are bounded.

a) Compactness of $W_2 := (T+\mu)^{-1}\, C_1^{(12)}\, (T+\mu)^{-1}$

We apply the strategy to write W_2 as the norm-convergent limit of a sequence $(W_{2n})_{n\in\mathbb{N}}$ of (compact) Hilbert-Schmidt operators. If so, W_2 is compact too.
In order to construct the Hilbert Schmidt operators we use the property that an operator A is Hilbert-Schmidt iff its kernel k_A is square integrable (Reed-Simon 1980, Theorem VI.23).

In order to define the sequence $(W_{2n})_{n\in\mathbb{N}}$, we must introduce convergence generating functions in momentum space and apply a regularisation of the Coulomb potential.

We first decompose $C_1^{(12)}$ into two self-adjoint operators,

$$C_1^{(12)} \;=\; C_{1\epsilon}^{(12)} \;+\; R_{1\epsilon}^{(12)}, \tag{II.6.14}$$

$$C_{1\epsilon}^{(12)} := \; e^{-\epsilon(p_1+p_2)} V^{(12)} \Lambda_-^{(1)} F_0^{(1)} \;+\; F_0^{(1)} \Lambda_-^{(1)} V^{(12)} e^{-\epsilon(p_1+p_2)}$$

$$R_{1\epsilon}^{(12)} := \; g_\epsilon V^{(12)} \Lambda_-^{(1)} F_0^{(1)} \;+\; F_0^{(1)} \Lambda_-^{(1)} V^{(12)} g_\epsilon, \qquad g_\epsilon := \; 1 \,-\, e^{-\epsilon(p_1+p_2)}$$

and secondly, we introduce the screened Coulomb field $\frac{1}{x}e^{-\epsilon x}$ with its Fourier transform $\sqrt{\frac{2}{\pi}}\,\frac{1}{p^2+\epsilon^2}$ and decompose each of the two momentum denominators in the prefactor of the kernel (II.4.10) of $C^{(12)}$ (which is twice the kernel of $C_1^{(12)}$) according to

$$\frac{1}{p^2} \;=\; e_\epsilon \,+\, f_\epsilon, \qquad e_\epsilon := \frac{1}{p^2+\epsilon^2}, \quad f_\epsilon := \frac{\epsilon^2}{p^2(p^2+\epsilon^2)} \tag{II.6.15}$$

which results in a decomposition of $C_1^{(12)}$ into 8 self-adjoint operators,

$$C_1^{(12)} \;=\; C_{1\epsilon}^{(12)}(e_\epsilon,e_\epsilon) \;+\; C_{1\epsilon}^{(12)}(e_\epsilon,f_\epsilon) \;+\; C_{1\epsilon}^{(12)}(f_\epsilon,e_\epsilon) \;+\; C_{1\epsilon}^{(12)}(f_\epsilon,f_\epsilon)$$

$$+\, R_{1\epsilon}^{(12)}(e_\epsilon,e_\epsilon) \;+\; R_{1\epsilon}^{(12)}(e_\epsilon,f_\epsilon) \;+\; R_{1\epsilon}^{(12)}(f_\epsilon,e_\epsilon) \;+\; R_{1\epsilon}^{(12)}(f_\epsilon,f_\epsilon). \tag{II.6.16}$$

We now prove the compactness of $W_{2n} := (T+\mu)^{-1}\, C_{1\epsilon}^{(12)}(e_\epsilon,e_\epsilon)\, (T+\mu)^{-1}$ with $\epsilon := 1/n$ via the square integrability of its kernel. Subsequently we will show that the remaining operators from the decomposition of $C_1^{(12)}$ vanish in the limit $\epsilon \to 0$. We have

$$k_{C_{1\epsilon}^{(12)}(e_\epsilon,e_\epsilon)}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2') \;=\; -\,\frac{\gamma e^2}{(2\pi)^4}\,\frac{1}{|\mathbf{p}_2-\mathbf{p}_2'|^2+\epsilon^2}\,\frac{1}{|\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1-\mathbf{p}_1'|^2+\epsilon^2} \tag{II.6.17}$$

$$\cdot\left\{ e^{-\epsilon(p_1+p_2)}\,\frac{1}{E_{|\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1|}+E_{p_1'}}\,(1-\tilde{D}_0^{(1)}(\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1'))\,(1+\tilde{D}_0^{(1)}(\mathbf{p}_1'))\right.$$

$$\left. +\,\frac{1}{E_{p_1}+E_{|\mathbf{p}_2'-\mathbf{p}_2+\mathbf{p}_1'|}}\,(1+\tilde{D}_0^{(1)}(\mathbf{p}_1))\,(1-\tilde{D}_0^{(1)}(\mathbf{p}_2'-\mathbf{p}_2+\mathbf{p}_1'))\,e^{-\epsilon(p_1'+p_2')}\right\}.$$

In the modulus of the kernel, $|1\pm\tilde{D}_0^{(1)}(\mathbf{p})|$ is estimated by 2 and the energy denominators by their massless expression, resulting in

$$|k_{W_{2n}}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2')| \le \frac{4\gamma e^2}{(2\pi)^4}\,\frac{1}{p_1+p_2+\mu}\,\frac{1}{|\mathbf{p}_2-\mathbf{p}_2'|^2+\epsilon^2}\,\frac{1}{|\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1-\mathbf{p}_1'|^2+\epsilon^2} \tag{II.6.18}$$

$$\cdot\left\{ e^{-\epsilon(p_1+p_2)}\,\frac{1}{|\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1|+p_1'} \;+\; \frac{1}{p_1+|\mathbf{p}_2'-\mathbf{p}_2+\mathbf{p}_1'|}\,e^{-\epsilon(p_1'+p_2')}\right\}\,\frac{1}{p_1'+p_2'+\mu}.$$

Using the substitutions $\mathbf{q}_2 := \mathbf{p}_2 - \mathbf{p}_2'$ and $\mathbf{q}_1 := \mathbf{p}_1 - \mathbf{p}_1' + \mathbf{q}_2$ as well as the estimates $(p_1 + p_2 + \mu)^{-1} \leq 1,\;\; (p_1' + p_2' + \mu)^{-1} \leq 1$ for $\mu \geq 1,$ we have to show that the integral S is finite, defined by

$$S := \int d\mathbf{p}_1\, d\mathbf{p}_2\, d\mathbf{p}_1'\, d\mathbf{p}_2'\, |k_{W_{2n}}(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p}_1', \mathbf{p}_2')|^2 \leq \frac{4\gamma e^2}{(2\pi)^4} \int d\mathbf{q}_1\, d\mathbf{q}_2 \qquad \text{(II.6.19)}$$

$$\cdot \frac{1}{(q_2^2+\epsilon^2)^2}\, \frac{1}{(q_1^2+\epsilon^2)^2} \left\{ \int d\mathbf{p}_1\, d\mathbf{p}_2\, e^{-2\epsilon(p_1+p_2)}\, \frac{1}{(|\mathbf{p}_1+\mathbf{q}_2| + |\mathbf{p}_1+\mathbf{q}_2-\mathbf{q}_1|)^2} \right.$$

$$+ \int d\mathbf{p}_1'\, d\mathbf{p}_2' \left(2e^{-\epsilon(|\mathbf{q}_1+\mathbf{p}_1'-\mathbf{q}_2| + |\mathbf{q}_2+\mathbf{p}_2'|)}\, e^{-\epsilon(p_1'+p_2')}\, \frac{1}{p_1' + |\mathbf{q}_1+\mathbf{p}_1'|} \right.$$

$$\left.\left. \cdot \frac{1}{|\mathbf{q}_1+\mathbf{p}_1'-\mathbf{q}_2| + |\mathbf{p}_1'-\mathbf{q}_2|} + e^{-2\epsilon(p_1'+p_2')}\, \frac{1}{(|\mathbf{q}_1+\mathbf{p}_1'-\mathbf{q}_2| + |\mathbf{p}_1'-\mathbf{q}_2|)^2} \right) \right\}.$$

It is obvious that for $\epsilon > 0$, all integrals converge near zero and infinity. Explicitly, in the first term (using the formulae from Appendix A)

$$\int d\mathbf{q}_2\, \frac{1}{(q_2^2+\epsilon^2)^2}\, \frac{1}{(|\mathbf{p}_1+\mathbf{q}_2| + |\mathbf{p}_1+\mathbf{q}_2-\mathbf{q}_1|)^2} \leq \int d\mathbf{q}_2\, \frac{1}{(q_2^2+\epsilon^2)^2}\, \frac{1}{|\mathbf{p}_1+\mathbf{q}_2|^2}$$

$$= \int_0^\infty \frac{q_2\, dq_2}{(q_2^2+\epsilon^2)^2}\, \frac{2\pi}{p_1}\, \ln \frac{q_2+p_1}{|q_2-p_1|} = \frac{c}{p_1} \qquad \text{(II.6.20)}$$

with $c < \infty$, and similarly for the third term. In the second term, the denominator is estimated by $(p_1' \cdot |\mathbf{p}_1' - \mathbf{q}_2|)^{-1}$ showing that this singularity is even weaker. This proves that W_{2n} is Hilbert-Schmidt.

It remains to show that $\|W_{2n} - W_2\| = \|(T+\mu)^{-1} \left(C_1^{(12)} - C_{1\epsilon}^{(12)}(e_\epsilon, e_\epsilon) \right) (T + \mu)^{-1}\| \to 0$ with $\epsilon \to 0$.

Since all seven contributions to $C_1^{(12)} - C_{1\epsilon}^{(12)}(e_\epsilon, e_\epsilon)$ are self-adjoint, each of these operators can be estimated separately with the help of the generalised Lieb and Yau formula and suitable convergence generating functions. Two basic facts are needed to show the estimate by some power of ϵ

- $$\int d\mathbf{q}_1\, \frac{\epsilon^2}{q_1^2(q_1^2+\epsilon^2)} = 4\pi\epsilon^2 \int_0^\infty \frac{dq_1}{q_1^2+\epsilon^2} = 2\pi^2\epsilon \qquad \text{(II.6.21)}$$
- $$\frac{1}{p+\mu}\left(1 - e^{-\epsilon p}\right) \leq \frac{1}{p}\left(1 - e^{-\epsilon p}\right) \leq \epsilon. \qquad \text{(II.6.22)}$$

The proof is displayed in Appendix D, with the result (for $m \neq 0$)

$$\|(W_{2n} - W_2)\, \psi\|^2 \leq c^2 \epsilon\, \|\psi\|^2 \qquad \text{(II.6.23)}$$

which proves that W_2 is Hilbert-Schmidt.

b) Boundedness of $(T+\mu)\,(H^{(2)}+\mu)^{-1}$

For $\chi \in \mathcal{A}(L_2(\mathbb{R}^3) \times \mathbb{C}^4)^2$ and $\psi := (H^{(2)}+\mu)^{-1}\chi \in \mathcal{A}(H^1(\mathbb{R}^3) \times \mathbb{C}^4)^2,$ we have to show that there exists a constant c such that

$$\|(T+\mu)\,(H^{(2)}+\mu)^{-1}\chi\|^2 = (\psi, (T+\mu)^2\,\psi) \overset{!}{\leq} c\,\|\chi\|^2 = c\,(\psi, (H^{(2)}+\mu)^2\,\psi) \qquad \text{(II.6.24)}$$

for some $\mu \geq 1$. Let $H^{(2)} = T + W$. We follow BBHS (1999) and use the triangle inequality, $\|(H^{(2)}+\mu)\psi\| \geq \|(T+\mu)\psi\| - \|W\psi\|$.

Assume we can show

$$\|W\,\psi\| \overset{!}{\leq} c_0\,\|T\,\psi\| \qquad \text{(II.6.25)}$$

with $c_0 < 1$. Then from $\|T\psi\| \leq \|(T+\mu)\psi\|$ we get

$$\|(H^{(2)}+\mu)\,\psi\| \geq (1-c_0)\,\|(T+\mu)\,\psi\|. \qquad \text{(II.6.26)}$$

From this inequality, (II.6.24) is a consequence if we require

$$\|(T+\mu)\,\psi\| \;\leq\; c\,(1-c_0)\;\|(T+\mu)\,\psi\| \tag{II.6.27}$$

which is fulfilled for $c \geq \dfrac{1}{1-c_0}$. We note that (II.6.25) has already been proven in the form sense (Proposition II.3); it does, however, not follow from (II.5.58), as is well known (Kadison and Ringrose 1983, p.251). In fact, potentials with Coulomb singularities have weaker estimates in the norm sense than in the form sense (see Appendix C).

Proof of (II.6.25):
Since the total potential enters quadratically, we have to use its symmetrised form (with respect to particle exchange), i.e. replace $2C_1^{(12)}$ by $C_1^{(12)}+C_2^{(12)}$. From the antisymmetry property of ψ together with the fact that for any pair of self-adjoint operators A,B one has $|(\psi,AB\,\psi)| = |(BA\,\psi,\psi)| = |(\psi,BA\,\psi)|$, the estimate of $\|W\psi\|^2 = (\psi,W^2\psi)$ can be reduced to

$$(\psi,\,(W^{(1)}\,+\,W^{(2)}\,+\,V^{(12)}\,+\,C_1^{(12)}\,+\,C_2^{(12)})^2\,\psi) \tag{II.6.28}$$

$$\leq\;(\psi,\,[(W^{(1)}+W^{(2)})^2\,+\,(V^{(12)})^2\,+\,2(C_1^{(12)})^2]\,\psi)\;+\;2\,|(\psi,C_1^{(12)}C_2^{(12)}\,\psi)|$$

$$+4|(\psi,W^{(1)}V^{(12)}\psi)|+4|(\psi,W^{(1)}C_1^{(12)}\psi)|+4|(\psi,W^{(1)}C_2^{(12)}\psi)|+4|(\psi,V^{(12)}C_1^{(12)}\psi)|.$$

Let us first consider the massless case. In Appendix C, the estimates for $(\psi,(W^{(1)})^2\psi)$ and $(\psi,(V^{(12)})^2\psi)$ are calculated, with the results

$$(\psi,(W^{(1)})^2\,\psi)\;\leq\;c_w\,(\psi,p_1^2\,\psi),\qquad c_w=\left(\frac{4}{3}\gamma+\frac{2}{9}\gamma^2\right)^2\;=\;(1.33\gamma+0.22\gamma^2)^2,$$

$$(\psi,(V^{(12)})^2\,\psi)\;\leq\;c_v\,(\psi,p_1^2\,\psi)\;=\;c_v\,(\psi,p_2^2\,\psi),\qquad c_v=4e^4. \tag{II.6.29}$$

Further, we estimate

$$\|C_1^{(12)}\,\psi\|\;\leq\;\|V^{(12)}\Lambda_-^{(1)}F_0^{(1)}\,\psi\|\;+\;\|F_0^{(1)}\Lambda_-^{(1)}V^{(12)}\,\psi\|$$

$$\leq\;\|V^{(12)}\Lambda_-^{(1)}F_0^{(1)}\,\psi\|\;+\;\|F_0^{(1)}\|\cdot\|\Lambda_-^{(1)}\|\cdot\|V^{(12)}\,\psi\|. \tag{II.6.30}$$

For the first term, define $\varphi := \Lambda_-^{(1)}F_0^{(1)}\psi$ and $\chi := p_2\psi$ (with $\chi\in\mathcal{A}(L_2(\mathbb{R}^3)\times\mathbb{C}^4)^2$, $\varphi,\psi\in\mathcal{A}(H_1(\mathbb{R}^3)\times\mathbb{C}^4)^2$) such that

$$\|V^{(12)}\Lambda_-^{(1)}F_0^{(1)}\,\psi\|\;=\;\|V^{(12)}\varphi\|\;\leq\;\sqrt{c_v}\,\|p_2\,\varphi\|\;=\;\sqrt{c_v}\,\|p_2\Lambda_-^{(1)}F_0^{(1)}\,\psi\|$$

$$=\;\sqrt{c_v}\,\|\Lambda_-^{(1)}F_0^{(1)}p_2\,\psi\|\;\leq\;\sqrt{c_v}\,\|\Lambda_-^{(1)}\|\,\|F_0^{(1)}\|\,\|p_2\,\psi\|\;\leq\;\sqrt{c_v}\,\|F_0^{(1)}\|\,(\psi,p_2^2\,\psi)^{\frac{1}{2}}. \tag{II.6.31}$$

From the estimate (II.5.22), $\|F_0^{(1)}\|\leq\frac{\gamma}{\pi}\,(\frac{\pi^2}{4}-1)$ and therefore

$$\|C_1^{(12)}\,\psi\|\;\leq\;\|F_0^{(1)}\|\,\left(\sqrt{c_v}\,(\psi,p_2^2\,\psi)^{\frac{1}{2}}\,+\,\|V^{(12)}\,\psi\|\right)\;\leq\;\sqrt{c_s}\,\|p_2\,\psi\|, \tag{II.6.32}$$

with $c_s = \left(\dfrac{2\gamma}{\pi}\left[\dfrac{\pi^2}{4}-1\right]\right)^2 c_v$.

Again from Appendix C, $|(\psi,W^{(1)}W^{(2)}\,\psi)|\leq c_n\,(\psi,p_1p_2\,\psi)$ with $c_n=[\frac{\gamma}{2}(\frac{\pi}{2}+\frac{2}{\pi})+\frac{\gamma^2}{8}(\frac{\pi}{2}-\frac{2}{\pi})^2]^2 = (1.1\gamma+0.11\gamma^2)^2 < c_w$ (for $\gamma>0$) , such that

$$(\psi,(W^{(1)}+W^{(2)})^2\,\psi)\;\leq\;2\,(\psi,(W^{(1)})^2\,\psi)\;+\;2\,|(\psi,W^{(1)}W^{(2)}\,\psi)|$$

$$\leq\;c_w\,(\psi,\,(p_1^2+p_2^2)\,\psi)\;+\;2c_n\,(\psi,p_1p_2\,\psi)\;\leq\;c_w\,(\psi,T^2\,\psi). \tag{II.6.33}$$

Since the estimates of $V^{(12)}$ and $C_1^{(12)}$, $C_2^{(2)}$ are smaller by a factor of e^2 as compared to those of $W^{(1)}$ and $W^{(2)}$ (when the central potential strength γ is large), we are not aiming at optimised estimates. Rather, we use estimates of the type (for A,B self-adjoint), $|(\psi,AB\psi)| = |(A\psi,B\psi)| \leq \|A\psi\|\cdot\|B\psi\|$.

As an exemplary case, consider

$$|(\psi, W^{(1)}V^{(12)}\,\psi)| \;\leq\; \|W^{(1)}\,\psi\|\;\|V^{(12)}\,\psi\| \;\leq\; \sqrt{c_w}\;\|p_1\,\psi\| \cdot \sqrt{c_v}\;\|p_2\,\psi\|$$

$$=\; \sqrt{c_w c_v}\;\|p_1\,\psi\|^2 \;=\; \frac{1}{2}\,\sqrt{c_w c_v}\;(\psi,\,(p_1^2+p_2^2)\,\psi) \;\leq\; \frac{1}{2}\,\sqrt{c_w c_v}\;(\psi, T^2\,\psi). \qquad \text{(II.6.34)}$$

Thus, collecting results,

$$(\psi, W^2\,\psi) \;\leq\; (c_w \,+\, 2e^4 \,+\, 2c_s \,+\, 4e^2\sqrt{c_w} \,+\, 4\sqrt{c_w c_s} \,+\, 4e^2\sqrt{c_s}\,)\;(\psi, T^2\,\psi)$$

$$=: c_0^2\;\|T\,\psi\|^2 \qquad \text{(II.6.35)}$$

with $c_0 < 1$ for $\gamma < 0.654$ $(Z \leq 89)$. Hence the boundedness of $(T+\mu)(H^{(2)}+\mu)^{-1}$ is proven for $m=0$ and $\gamma < 0.654$.

We follow the argumentation of Herbst (1977) to infer the boundedness for the $m \neq 0$ case, with the same bound. The only necessary ingredient to show is the scaling property of $(T+\mu)(H^{(2)}+\mu)^{-1}$ under dilations.

First we note that no specification of μ was needed in the $m=0$ proof of the boundedness. Since $T = \sqrt{p_1^2+m^2} + \sqrt{p_2^2+m^2} > 0$ for $m \neq 0$ and, according to Proposition II.3, $H^{(2)} > 0$ for $\gamma < 0.825$ which is larger than the critical γ from above, both T and $H^{(2)}$ are invertible such that μ can be set to zero. In the compactness proof, μ can also be set to zero if $m \neq 0$. The reason is the estimate $\dfrac{1}{\sqrt{p^2+m^2}} \leq \dfrac{c}{p+1}$ for a suitable constant c (e.g. $c \geq \max\{2, \frac{2}{m}\}$). Since the values of the occurring bounds are irrelevant, a finite additional factor c plays no role.

We introduce the dilation d_θ by means of $d_\theta\hat{\psi}(\mathbf{p}_1,\mathbf{p}_2) = \theta^{-3}\,\hat{\psi}(\mathbf{p}_1/\theta,\mathbf{p}_2/\theta)$ $=: \hat{\psi}_\theta(\mathbf{p}_1,\mathbf{p}_2)$ for $\theta \in \mathbb{R}_+$.

From (I.5.5) we know that $d_\theta E_p(m)\,d_\theta^{-1} = E_{p/\theta}(m) = \frac{1}{\theta}\,E_p(m\cdot\theta)$. Similarly, $d_\theta W^{(k)}(m)\,d_\theta^{-1} = \frac{1}{\theta}W^{(k)}(m\cdot\theta)$, $k=1,2$ follows from the scaling properties of b_{km} because of (I.4.1) and $d_\theta U_0'(m)d_\theta^{-1} = U_0'(m\cdot\theta)$ (which is easily obtained from the explicit expression (I.3.1) for U_0').

For the two-particle operators $V^{(12)}$ and $C_1^{(12)}$ one has from (II.4.8) – (II.4.11),

$$(\psi, V^{(12)}\,\psi) \;=\; (\psi_\theta, d_\theta V^{(12)} d_\theta^{-1}\,\psi_\theta) \qquad \text{(II.6.36)}$$

$$=\; \int d\mathbf{p}_1\,d\mathbf{p}_2\,\theta^{-3}\hat{\psi}(\mathbf{p}_1/\theta,\mathbf{p}_2/\theta) \int d\mathbf{p}_1'\,d\mathbf{p}_2'\,k_\theta(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2')\,\theta^{-3}\,\hat{\psi}(\mathbf{p}_1'/\theta,\mathbf{p}_2'/\theta)$$

$$=\; \theta^6 \int d\mathbf{p}_1/\theta\,d\mathbf{p}_2/\theta\,\hat{\psi}(\mathbf{p}_1/\theta,\mathbf{p}_2/\theta) \int d\mathbf{p}_1'/\theta\,d\mathbf{p}_2'/\theta\,k_\theta(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2')\,\hat{\psi}(\mathbf{p}_1'/\theta,\mathbf{p}_2'/\theta)$$

where $k_\theta = d_\theta\,k\,d_\theta^{-1}$ is the dilated kernel of $V^{(12)}$ (respective $C_1^{(12)}$).

Upon considering $d\mathbf{p}_k/\theta$, $d\mathbf{p}_k'/\theta$, $k=1,2$ as new variables, one can identify

$$k(\mathbf{p}_1/\theta,\mathbf{p}_2/\theta;\mathbf{p}_1'/\theta,\mathbf{p}_2'/\theta)\;\theta^{-6} \;=\; k_\theta(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2'). \qquad \text{(II.6.37)}$$

Thus one easily verifies from the explicit form (II.4.11), (II.4.10) of the kernels of $V^{(12)}$ and $C_1^{(12)}$, that $k_{V^{(12)},\theta}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2') = \frac{1}{\theta}\,k_{V^{(12)}}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2')$ and $(d_\theta k_{C^{(12)},m} d_\theta^{-1})(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2') = \frac{1}{\theta}\,k_{C^{(12)},m\cdot\theta}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2')$. Hence we have

$$d_\theta\,H^{(2)}(m)\,d_\theta^{-1} \;=\; \frac{1}{\theta}\;H^{(2)}(m\cdot\theta), \qquad d_\theta\,T(m)\,d_\theta^{-1} \;=\; \frac{1}{\theta}\,T(m\cdot\theta). \qquad \text{(II.6.38)}$$

Moreover, with $H_\theta^{(2)} = \frac{1}{\theta}\,H^{(2)}(m\cdot\theta)$ it follows upon inversion that $(H_\theta^{(2)})^{-1} = (\frac{1}{\theta}\,H^{(2)}(m\cdot\theta))^{-1} = \theta\,(H^{(2)}(m\cdot\theta))^{-1}$. Thus

$$d_\theta\,T\,(H^{(2)})^{-1}\,d_\theta^{-1} \;=\; (d_\theta\,T\,d_\theta^{-1})\,(d_\theta\,H^{(2)}\,d_\theta^{-1})^{-1} \;=\; \frac{1}{\theta}\,T(m\cdot\theta)\cdot\theta\,(H^{(2)}(m\cdot\theta))^{-1}$$

$$=\; T\,(H^{(2)})^{-1}(m\cdot\theta). \qquad \text{(II.6.39)}$$

Hence our operator is dilational invariant with m being absorbed in the dilation parameter $\theta' := m \cdot \theta$. Since dilation as a unitary transformation does not change the norm, we get $\|T\,(H^{(2)})^{-1}(m)\| = \|T\,(H^{(2)})^{-1}(m=0)\| \le c$ with the constant c from the $m = 0$ estimate given above.

c) Boundedness of $(H_v + \mu)^{-1}(T + \mu)$

From Lemma I.4 we have $\|(H_v+\mu)^{-1}\,(T+\mu)\| \le c$ if $\|(T+\mu)\,(H_v+\mu)^{-1}\| \le c$. However, for $\gamma < 0.654$, the latter follows immediately from the proof of boundedness of $(T+\mu)(H^{(2)}+\mu)^{-1}$ upon dropping the interactions $C_1^{(12)},\ C_2^{(12)}$ everywhere. ■

It should be noted that in the r.h.s of (II.6.7) in Theorem II.1, the electron-electron interaction $V^{(12)}$ cannot be dropped. In fact, its kernel contains the delta-function (viz. (II.4.11)), the square of which is highly singular. The fact that $V^{(12)}$ is not relatively compact with respect to T is due to the unboundedness of $V^{(12)}$ when x_1 and x_2 go to infinity, keeping simultaneously $\mathbf{x}_1 = \mathbf{x}_2$ (Reed-Simon 1978, p.120).

Concerning the absence of eigenvalues in the massless case, the same holds true as in the one-particle case.

Theorem II.2 (Absence of eigenvalues in massless case).
Let $m = 0$ and the critical potential strength $\gamma_0 = 0.986$ as in Proposition II.3. Then the spectrum of $H^{(2)}$ has no eigenvalues for $\gamma < \gamma_0$.

Proof. We show that (i), $H^{(2)}$ has no eigenvalues $\neq 0$, and (ii) that $E = 0$ is no eigenvalue.

For (i) we argue as in the one-particle case (Theorem I.3(iii)). From (II.6.38) we know that $H^{(2)}$ scales under dilations according to $d_\theta H^{(2)}(m=0)\,d_\theta^{-1} = \frac{1}{\theta}\,H^{(2)}(m=0)$. Therefore, assume ψ is an eigenfunction of $H^{(2)}$ with eigenvalue $E \neq 0$, then $d_\theta\psi$ is also an eigenfunction of $H^{(2)}$ (with eigenvalue θE). This contradicts the separability of the Hilbert space $(H_{1/2}(\mathbb{R})^3 \times \mathbb{C}^4)^2$.

For (ii) we also follow the proof of Theorem I.3(iii). Assume there exists an eigenfunction $\psi \neq 0$ to $H^{(2)}$ with eigenvalue $E = 0$. Then from (II.5.61) and a partial wave analysis, together with the Mellin transform properties given in BSS (2002), see Appendix C for a generalisation to the two-particle case, we have

$$0 \;=\; (\psi, H^{(2)}\,\psi) \;\ge\; \left(1 \,-\, \gamma\,(\frac{1}{\gamma_{BR}} \,+\, e^2\,\frac{\pi^2}{4}\,) \,+\, d\,\gamma^2\right)\;(\psi, 2p_1\,\psi)$$
$$=\; 2\int d\mathbf{p}_2\,\sum_\nu \int_{-\infty}^{\infty} dt\;\left|a^{\#}_{\nu,p_2}(t+i/2)\right|^2\;\left(1 \,-\, \gamma\,(\frac{1}{\gamma_{BR}} \,+\, e^2\,\frac{\pi^2}{4}\,) \,+\, d\,\gamma^2\right). \tag{II.6.40}$$

If $\gamma < 0.986$, the factor in brackets is strictly positive and hence $|a^{\#}_{\nu,p_2}(t+\frac{i}{2})|^2 = 0$ almost everywhere. The remaining part of the proof can be copied from the one of Theorem I.3(iii), to show that $\psi = 0$, a contradiction. ■

III. Outlook: The general N-particle case

For N fermionic particles, we define the positive spectral subspace of the free N-particle Dirac operator by means of $\mathcal{H}_{+,N} := \Lambda_{+,N}\,\mathcal{A}\left(H_{1/2}(\mathbb{R}^3)\times\mathbb{C}^4\right)^N$, to be considered as subspace of the Hilbert space $\Lambda_{+,N}\mathcal{A}(L_2(\mathbb{R}^3)\times\mathbb{C}^4)^N$, where $\Lambda_{+,N}$ is the product of the free projectors for each particle,

$$\Lambda_{+,N} := \Lambda_+^{(1)}\cdots\Lambda_+^{(N)}. \tag{III.1}$$

and the spin of each particle is assumed to be $\frac{1}{2}$. A state $\psi\in\mathcal{H}_{+,N}$ can be considered as a superposition of Slater determinants (see section II.1), such that each summand of ψ contains a product of N one-particle states, $\prod_{i=1}^{N}\varphi_{\sigma(i)}^{(\alpha)}(\mathbf{x}_i)$, where $\sigma\in S_N$ is a permutation and α enumerates the basis of the single-particle Hamiltonian $h^{(k)}$. Since operators acting on distinct particles commute, the above definition of our Hilbert space agrees with the conventional definition $\mathcal{H}_{+,N} = \Lambda_{n=1}^N\mathcal{H}_+$ where $\Lambda_{n=1}^N$ symbolises the N-fold antisymmetric tensor product of the single-particle Hilbert spaces $\mathcal{H}_+ := \Lambda_+\,(H_{1/2}(\mathbb{R}^3)\times\mathbb{C}^4)$ (see e.g. Hoever and Siedentop 1999). In particular, one has $\Lambda_+^{(k)}\psi=\psi$ for all $k=1,...,N$.

The transformation scheme for the Coulomb-Dirac operator (II.1), introduced in section II.2 for the two-particle case, can readily be generalised to an atom with N electrons, $N>2$. Iterating the representation (II.2.5) of the projector $P_+^{(k)}$ for particle k, to get $P_+^{(k)} = \Lambda_+^{(k)} + F_0^{(k)} + R((e^2)^2)$, and defining the products

$$\mathcal{F}_k := \Lambda_+^{(1)}\cdots\Lambda_+^{(k-1)}\,F_0^{(k)}\,\Lambda_+^{(k+1)}\cdots\Lambda_+^{(N)}, \qquad k\in\{1,...,N\}, \tag{III.2}$$

the two-particle interaction term of (II.1) is expanded according to

$$P_{+,N}\sum_{n<k}^{N}V^{(nk)}\,P_{+,N} \;=\; \sum_{n<k}^{N}\Big(\Lambda_+^{(n)}\Lambda_+^{(k)}\,V^{(nk)}\,\Lambda_{+,N}$$
$$+\;\sum_{\substack{m=1\\ m\neq n,k}}^{N}(\Lambda_+^{(n)}\Lambda_+^{(k)}\,V^{(nk)}\,\Lambda_+^{(m)}\,\mathcal{F}_m \;+\; \mathcal{F}_m\,\Lambda_+^{(m)}\,V^{(nk)}\,\Lambda_+^{(n)}\,\Lambda_+^{(k)})$$
$$+\,F_0^{(n)}\,\Lambda_+^{(k)}\,V^{(nk)}\,\Lambda_{+,N} \;+\; F_0^{(k)}\,\Lambda_+^{(n)}\,V^{(nk)}\,\Lambda_{+,N} \;+\; \Lambda_{+,N}\,V^{(nk)}\,F_0^{(n)}\,\Lambda_+^{(k)} \tag{III.3}$$
$$+\,\Lambda_{+,N}\,V^{(nk)}\,F_0^{(k)}\,\Lambda_+^{(n)}\Big) \;+\; R((e^2)^3).$$

The first Sobolev transformation can be written in terms of the one-particle self-adjoint operators $B_1^{(k)}$

$$U_1 = e^{iB_1}, \qquad B_1 \;=\; \sum_{k=1}^{N}B_1^{(k)}. \tag{III.4}$$

Then the Coulomb-Dirac operator turns into

$$U_1^{-1}\,H\,U_1 \;=\; \sum_{k=1}^{N}\left(D_0^{(k)} \;+\; V_1^{(k)} \;+\; i[V_1^{(k)},B_1^{(k)}] \;+\; \frac{i}{2}\,[W_1^{(k)},B_1^{(k)}]\right)$$
$$+\;\sum_{n<k}^{N}\Big\{\Lambda_+^{(n)}\,\Lambda_+^{(k)}\,V^{(nk)}\,\Lambda_{+,N} \;+\; i\,[\Lambda_+^{(n)}\,\Lambda_+^{(k)}\,V^{(nk)}\Lambda_{+,N},B_1^{(1)}+...+B_1^{(N)}] \tag{III.5}$$
$$+\;\sum_{\substack{m=1\\ m\neq n,k}}^{N}\Big(\Lambda_+^{(n)}\Lambda_+^{(k)}V^{(nk)}\,\Lambda_+^{(m)}\,\mathcal{F}_m \;+\; \mathcal{F}_m\,\Lambda_+^{(m)}\,V^{(nk)}\,\Lambda_+^{(n)}\,\Lambda_+^{(k)}\Big)$$

$$+\left(F_0^{(n)}\Lambda_+^{(k)}+F_0^{(k)}\Lambda_+^{(n)}\right)V^{(nk)}\Lambda_{+,N}+\Lambda_{+,N}V^{(nk)}\left(F_0^{(n)}\Lambda_+^{(k)}+F_0^{(k)}\Lambda_+^{(n)}\right)\Big\}$$
$$+\ R((e^2)^3).$$

The second Sobolev transformation, $U_2=e^{iB_2}$, $B_2=\sum\limits_{k=1}^{N}B_2^{(k)}+\sum\limits_{\mu}B_2^{(\mu)}+\sum\limits_{\lambda}B_2^{(\lambda)}$ with $B_2^{(k)}$ single-particle operators, $B_2^{(\mu)}$ two-particle and $B_2^{(\lambda)}$ three-particle operators (μ and λ running over all possible pairs and triplets that can be formed from N particles), eliminates the 'odd' second-order terms which have the form $\text{off}(C)=C-\text{proj}(C)$, $\text{proj}(C)$ collecting the block-diagonal terms in the three-particle representation of $C=1\cdot C\cdot 1$ with $1=(\Lambda_+^{(n)}+\Lambda_-^{(n)})(\Lambda_+^{(k)}+\Lambda_-^{(k)})(\Lambda_+^{(m)}+\Lambda_-^{(m)})$. The existence and boundedness of B_2 may be shown along the same lines as for the two-particle case.

Let us consider the expectation value of the transformed Hamiltonian with an N-particle wavefunction $\psi\in\mathcal{H}_{+,N}$. Disregarding positive projectors adjacent to ψ one obtains up to second order

$$(\psi,U_2^{-1}\,U_1^{-1}\,H\,U_1\,U_2\,\psi)\ =\ \sum_{k=1}^{N}\left(\psi,(D_0^{(k)}\ +\ V^{(k)}\ +\ \frac{i}{2}\,[W_1^{(k)},B_1^{(k)}]\,)\,\psi\right)$$
$$+\ \sum_{n<k}^{N}(\psi,H_{nk}\,\psi)\ +\ R((e^2)^3) \tag{III.6}$$

with

$$H_{nk}:=\ V^{(nk)}\ +\ i\,\{V^{(nk)}\,\Lambda_+^{(n)}\,B_1^{(n)}\ +\ V^{(nk)}\,\Lambda_+^{(k)}\,B_1^{(k)}\ -\ B_1^{(n)}\,\Lambda_+^{(n)}\,V^{(nk)}$$
$$-\ B_1^{(k)}\,\Lambda_+^{(k)}\,V^{(nk)}\ \}\ +\ V^{(nk)}\,F_0^{(n)}\ +\ V^{(nk)}\,F_0^{(k)}$$
$$+\ 2\sum_{\substack{m=1\\ m\neq k,n}}^{N}V^{(nk)}\,F_0^{(m)}\ +\ F_0^{(n)}\,V^{(nk)}\ +\ F_0^{(k)}\,V^{(nk)}. \tag{III.7}$$

Representing $B_1^{(k)}$ in terms of $F_0^{(k)}$ with the help of (II.3.21), H_{nk} simplifies to

$$H_{nk}\ =\ V^{(nk)}\ +\ V^{(nk)}\,(\Lambda_-^{(n)}\,F_0^{(n)}\ +\ \Lambda_-^{(k)}\,F_0^{(k)})\ +\ (F_0^{(n)}\,\Lambda_-^{(n)}\ +\ F_0^{(k)}\,\Lambda_-^{(k)})\,V^{(nk)}$$
$$+\ 2\sum_{\substack{m=1\\ m\neq n,k}}^{N}V^{(nk)}\,F_0^{(m)}. \tag{III.8}$$

Since in the last term of (III.8), the two operators $V^{(nk)}$ and $F_0^{(m)}$ act on distinct particles, it can be shown that this term vanishes for $\psi\in\mathcal{H}_{+,N}$ (see Appendix J). Thus we obtain a simple generalisation of the transformed two-particle operator (II.4.4).

In principle, like in the one-particle case, an n-fold transformation of the Coulomb-Dirac operator will lead to an operator of the form $\text{proj}(A)+R((e^2)^{n+1})$ where $\text{proj}(A)$ is a generalisation of (II.2.2) which involves the diagonal products of n projectors. In $\text{proj}(A)$, up to n particles (out of N) are affected simultaneously.

We close our work with some results about the stability of the N-electron atom ($N\geq 3$).

Having found the Sobolev representation of the transformed (up to second order) N-particle Coulomb-Dirac operator $H^{(2)}$ we can use the results from part I and II to establish a lower bound.

Let

$$(\psi, H^{(2)}\,\psi) \;=\; \sum_{k=1}^{N}(\psi, B_m^{(k)}\,\psi) \;+\; \sum_{k>n}^{N}(\psi,\,(V^{(nk)} \;+\; C^{(nk)})\,\psi) \tag{III.9}$$

where the operators on the r.h.s. of (III.6) and (III.8) are abbreviated by $B_m^{(k)}$, the Jansen-Hess operator of particle k, and $C^{(nk)}$, the second-order interaction between particles n and k.

From Proposition I.5 we have

$$(\psi, B_m^{(k)}\,\psi) \;\geq\; c(\gamma)\;(\psi, D_0^{(k)}\,\psi) \tag{III.10}$$

with $c(\gamma) \,=1-\frac{\gamma}{\gamma_{BR}} - \frac{\gamma^2}{8}(\frac{\pi}{2}-\frac{2}{\pi})^2$ from (I.4.53), where we have used that $\psi \in \mathcal{H}_{+,N}$ such that $E^{(k)}\psi = D_0^{(k)}\psi$.

Moreover, the second-order two-particle potential is estimated from Lemma II.4,

$$|(\psi, C^{(nk)}\,\psi)| \;\leq\; \gamma e^2\,\frac{\pi^2}{4}\,(\psi,\,(D_0^{(n)} \;+\; D_0^{(k)})\,\psi) \;=\; \gamma e^2\,\frac{\pi^2}{2}\,(\psi, D_0^{(1)}\,\psi) \tag{III.11}$$

where the symmetry of $\overline{\psi}\psi$ with respect to particle exchange has been exploited. Hence $\sum\limits_{k>n}^{N} \;=\; \frac{N(N-1)}{2}$ can be used, together with $(\psi, N D_0^{(1)}\,\psi) \;=\; \sum\limits_{k=1}^{N}(\psi, D_0^{(k)}\,\psi)$. Finally one can take advantage of $V^{(nk)} \geq 0$ to drop the respective term.

Therefore, the total operator $H^{(2)}$ can be estimated by

$$(\psi, H^{(2)}\,\psi) \;\geq\; \sum_{k=1}^{N}(\psi,\,\left[c(\gamma) \;-\; \gamma e^2\,\frac{\pi^2(N-1)}{4}\right]\;D_0^{(k)}\,\psi). \tag{III.12}$$

We have stability, even positivity, for all γ for which the expression in square brackets is nonnegative.

Thus we have proved

Proposition III.1 (Stability of N-electron ions and atoms)**.**
Let $\gamma = Ze^2$, $N \leq Z$ be the number of electrons, and let $H^{(2)}$ be the transformed N-particle Coulomb-Dirac operator up to second order in the potential strength γ. Then

$$H^{(2)} \;\geq\; 0 \qquad\qquad \text{for } \gamma \;\leq\; \gamma_N \tag{III.13}$$

with γ_N the smallest solution to

$$1 \;-\; \frac{\gamma}{\gamma_{BR}} \;-\; \frac{\gamma^2}{8}\left(\frac{\pi}{2} \;-\; \frac{2}{\pi}\right)^2 \;-\; \gamma e^2\,\frac{\pi^2(N-1)}{4} \;=\; 0 \tag{III.14}$$

where $\gamma_{BR} = \frac{2}{\pi/2+2/\pi}$.
For neutral atoms ($N = Z$) we have stability for $\gamma \leq 0.446$ ($Z \leq 61$).

Since the l.h.s. of (III.14) is decreasing both with N and γ, it follows that for $\gamma \leq 0.446$, we have stability for all ions with $N \leq Z$.

Alternatively, one might think of estimating $C^{(nk)}$ by $V^{(nk)}$ via Proposition II.2. However, even with the conjecture $C = 1$, one would need the restriction $\gamma \leq \frac{1}{\pi}$ (i.e. $Z \leq 43$) for a positive two-particle interaction term. This bound is lower than the above value, $Z \leq 61$.

We remark that stability of matter for the Brown-Ravenhall operator was shown by Balinsky and Evans (1999) in the case of K nuclei and one electron, and by Hoever and Siedentop (1999) in the case of K nuclei and N electrons (at zero mass) for $\gamma \leq \gamma_{BR}$ ($Z \leq 124$) and $\gamma \leq 0.64$ ($Z \leq 88$), respectively.

The contribution of two-particle second-order terms (neglected in the Brown-Ravenhall operator) is usually considered to be unimportant because of the smallness of their coupling constant e^2 (with respect to γ). However, since these terms tend to be negative (which we conjecture from the negativity property of the kernel of $C^{(nk)}$, see (II.4.10)), and since they occur with a weight proportional to N^2, they will counteract stability for large N in a non-negligible way. That becomes evident from the large reduction of the critical potential strength for atoms as compared to one- or two-electron ions found in this work.

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Appendix A

Compilation of integrals

Let $\int\limits_{\mathbb{R}^3} d\mathbf{p} \;=\; \int\limits_0^\infty p^2 dp \int\limits_{S^2} d\omega$ with $\int\limits_{S^2} d\omega \;=\; 2\pi \int\limits_{-1}^{1} d(\cos\vartheta_p)$ in spherical coordinates, where ϑ_p is the azimuthal angle of $\mathbf{p}$ with respect to some fixed axis, assuming cylindrical symmetry.

We identify $(\mathbf{p}' \pm \mathbf{p})^2 \;= p'^2 + p^2 \pm 2pp' \cos\vartheta_{p'} \;=: b + ax$ with $x := \cos\vartheta_{p'}$ and $a := \pm 2pp'$, $\;b := p'^2 + p^2$.

$$\int_{S^2} d\omega' \, \frac{1}{|\mathbf{p}' \pm \mathbf{p}|^2} \;=\; \frac{2\pi}{pp'} \, \ln\left|\frac{p+p'}{p-p'}\right| \;=\; \frac{2\pi}{pp'} \begin{cases} \frac{2p}{p'} \;+\; O(p^2), & p \to 0 \\ \frac{2p'}{p} \;+\; O(\frac{1}{p^2}), & p \to \infty \end{cases} \tag{A.1}$$

$$\frac{1}{2\pi} \int_{S^2} d\omega' \, \frac{1}{|\mathbf{p}' \pm \mathbf{p}|} \, \frac{1}{(|\mathbf{p}' \pm \mathbf{p}| + c)^2} \;=\; \int_{-1}^{1} dx \, \frac{1}{\sqrt{b+ax}} \, \frac{1}{(\sqrt{b+ax} \; + c)^2}$$

$$= \; \frac{2}{a} \int_{\sqrt{b-a}}^{\sqrt{b+a}} \frac{dz}{(z+c)^2} \;=\; \frac{2}{a} \left(\frac{1}{\sqrt{b-a}+c} \;-\; \frac{1}{\sqrt{b+a}+c} \right). \tag{A.2}$$

As a by-product,

$$\int_{S^2} d\omega' \, \frac{1}{|\mathbf{p} \pm \mathbf{p}'|} \;=\; \frac{2\pi}{pp'} \, (p + p' \,-\, |p-p'|\,). \tag{A.3}$$

In the following integrals, $q_0(p'/p) := \ln \dfrac{p+p'}{|p-p'|} \;= \ln \dfrac{1+p'/p}{|1-p'/p|}$

and $q_1(y) := \dfrac{1}{2}(y + \dfrac{1}{y}) \, \ln \dfrac{1+y}{|1-y|} \; - 1.$

$$\frac{1}{2\pi} \int d\mathbf{p}' \, \frac{1}{|\mathbf{p}' \pm \mathbf{p}|^2} \, \frac{p}{p'^2} \;=\; \int_0^\infty \frac{dp'}{p'} \, \ln \frac{p+p'}{|p-p'|} \;=\; 2 \int_0^1 \frac{dy}{y} \, q_0(y) \;=\; \frac{\pi^2}{2} \tag{A.4}$$

$$\frac{1}{2\pi} \int d\mathbf{p}' \, \frac{1}{|\mathbf{p}' \pm \mathbf{p}|^2} \, \frac{p}{p'(p'+p)} \;=\; \int_0^\infty \frac{dp'}{p'+p} \, q_0(p/p') \;=\; \int_0^1 \frac{dy}{y} \, q_0(y) \;=\; \frac{\pi^2}{4} \tag{A.5}$$

$$\frac{1}{2\pi} \int d\mathbf{p}' \, \frac{1}{|\mathbf{p}' \pm \mathbf{p}|^2} \, \frac{p^2}{p'^2} \, \frac{1}{p'+p} \;=\; p \int_0^\infty \frac{dp'}{p'} \, \frac{1}{p'+p} \, q_0(p'/p) \;=\; \int_0^1 \frac{dy}{y} \, q_0(y) \;=\; \frac{\pi^2}{4} \tag{A.6}$$

$$\int_0^\infty \frac{dy}{y^\alpha} \, q_0(y) \;=\; \frac{\pi}{2} \, \frac{\Gamma(\frac{\alpha}{2}) \, \Gamma(1-\frac{\alpha}{2})}{\Gamma(\frac{\alpha+1}{2}) \, \Gamma(\frac{3-\alpha}{2})}, \qquad 0 < \alpha < 2 \tag{A.7}$$

$$\int_0^\infty \frac{dy}{\sqrt{y}} \, q_l(y) \;=\; \frac{2\pi}{2l+1}, \qquad l = 0, 1, ... \tag{A.8}$$

$$\int_0^\infty \frac{dp'}{p'} \, q_1(p/p') \;=\; 2 \int_0^1 \frac{dy}{y} \, q_1(y) \;=\; 2 \tag{A.9}$$

$$\int_0^\infty \frac{dp'}{p'+p} \, q_1(p/p') \;=\; \int_0^1 \frac{dy}{y} \, q_1(y) \;=\; 1. \tag{A.10}$$

The integrals can be found with the help of Gradshteyn and Ryzhik (1965); the integrals (A.4) and (A.9) are provided by EPS (1996), (A.7) by BSS (2002), while (A.8) is based on an integral given by Tix (1998; see also (C.6) and (C.7)).

We also provide some finite integrals which are needed for the proof of Theorem I.4. For $a>0$,

$$\int_0^a dy\, y^{5/2}\, q_0(y) \;=\; \frac{2}{7}\left[a^{\frac{7}{2}}\ln\left|\frac{1+a}{1-a}\right| - 2\arctan\sqrt{a} + 4\sqrt{a} + \frac{4}{5}\,a^{\frac{5}{2}} - \ln\left|\frac{1+\sqrt{a}}{1-\sqrt{a}}\right|\right] \tag{A.11}$$

$$\int_0^a dy\; y^{3/2}\; q_0(y) \;=\; \frac{2}{5}\left[a^{5/2}\ln\left|\frac{1+a}{1-a}\right| \;+\; \frac{4}{3}\,a^{3/2} \;+\; 2\arctan\sqrt{a} \;-\; \ln\left|\frac{\sqrt{a}+1}{\sqrt{a}-1}\right|\right] \tag{A.12}$$

$$\int_0^a dy\; y^{1/2}\; q_0(y) \;=\; \frac{2}{3}\left[a^{3/2}\ln\left|\frac{1+a}{1-a}\right| \;+\; 4\sqrt{a} \;-\; 2\arctan\sqrt{a} \;-\; \ln\left|\frac{1+\sqrt{a}}{1-\sqrt{a}}\right|\right] \tag{A.13}$$

$$\int_0^a dy\; \frac{1}{\sqrt{y}}\; q_0(y) \;=\; 2\sqrt{a}\;\ln\left|\frac{1+a}{1-a}\right| \;+\; 4\arctan\sqrt{a} \;-\; 2\ln\left|\frac{\sqrt{a}+1}{\sqrt{a}-1}\right| \tag{A.14}$$

$$\int_a^\infty dy\; \frac{1}{\sqrt{y}}\; q_0(y) \;=\; 2\left[\pi \;-\; \sqrt{a}\ln\left|\frac{1+a}{1-a}\right| \;-\; 2\arctan\sqrt{a} \;+\; \ln\left|\frac{\sqrt{a}+1}{\sqrt{a}-1}\right|\right] \tag{A.15}$$

$$\int_0^a dy\; \frac{1}{y^{3/2}}\; q_0(y) \;=\; 4\arctan\sqrt{a} \;+\; 2\ln\left|\frac{1+\sqrt{a}}{1-\sqrt{a}}\right| \;-\; \frac{2}{\sqrt{a}}\;\ln\left|\frac{1+a}{1-a}\right| \tag{A.16}$$

$$\int_a^\infty dy\; \frac{1}{y^{3/2}}\; q_0(y) \;=\; 2\pi \;-\; 2\ln\left|\frac{\sqrt{a}+1}{\sqrt{a}-1}\right| \;-\; 4\arctan\sqrt{a} \;+\; \frac{2}{\sqrt{a}}\;\ln\left|\frac{1+a}{1-a}\right| \tag{A.17}$$

$$\int_a^\infty dy\, \frac{1}{y^{5/2}}\, q_0(y) = \frac{2}{3}\left[-\pi + \frac{4}{\sqrt{a}} + 2\arctan\sqrt{a} + \frac{1}{a^{\frac{3}{2}}}\;\ln\left|\frac{1+a}{1-a}\right| - \ln\left|\frac{1+\sqrt{a}}{1-\sqrt{a}}\right|\right] \tag{A.18}$$

These integrals can be found in Gradshteyn and Ryzhik (1965, p.205,206), after substitutions of the type $x := 1/q,\;\; x := q^{1/2}$. Note that the integrals (A.11) – (A.13) diverge for $a\to\infty$, whereas (A.14) and (A.16) tend to 2π. For $a \to 0$, (A.18) diverges, too.

Appendix B

Partial-wave decomposition of the Jansen-Hess operator and its Mellin transform in the massless case

We provide a compilation of results given in EPS (1996), Tix (1997), Stockmeyer (2002) and BSS (2002).

a) Partial-wave decomposition for $m \geq 0$

For $u \in \mathcal{S}(\mathbb{R}^3)\times\mathbb{C}^2$ and for the Fourier transformed Coulomb field one introduces the partial wave expansions

$$\hat{u}(\mathbf{p}) \;=\; \sum_{\nu\in I} p^{-1}\, a_\nu(p)\; \Omega_\nu(\hat{\mathbf{p}}) \qquad\qquad \nu = \{l, M, s\}$$

$$\frac{1}{|\mathbf{p}-\mathbf{p}'|^2} \;=\; \frac{2\pi}{pp'}\;\sum_{lM} q_l(\frac{p}{p'})\;\overline{Y_{lM}(\hat{\mathbf{p}})}\;Y_{lM}(\hat{\mathbf{p}}') \tag{B.1}$$

where $\Omega_\nu(\hat{\mathbf{p}})$ are the Dirac angular momentum eigenstates (the vector spherical hamonics (Rose 1961)), $Y_{lM}(\hat{\mathbf{p}})$ are spherical harmonics and the reduced Legendre functions $q_l(x)$ are related to the Legendre functions $Q_l(x)$ of the second kind (Abramowitz and Stegun 1965) by $q_l(x) := \; Q_l(\frac{1}{2}x \;+\frac{1}{2x})$. For $x \neq 1$, one has the integral representation (EPS 1996)

$$q_l(x) \;=\; \int_{t+\sqrt{t^2-1}}^{\infty} \frac{z^{-l-1}\;dz}{\sqrt{1-2zt+z^2}}, \qquad\qquad t \;=\; \frac{1}{2}\,(x+\frac{1}{x}). \tag{B.2}$$

The index set is $I := \{\nu = (l,M,s)\,|\, l \in \mathbb{N}_0,\; M = -l-\frac{1}{2},...,l+\frac{1}{2},\; s = \pm\frac{1}{2},\; l+s > 0,\; \Omega_\nu \neq 0\}$ and $\hat{\mathbf{p}} := \mathbf{p}/p$. Then the expectation value $(u, b_m\, u)$ of the Jansen-Hess operator can be written in the following way, making use of the orthonormality of the set $\Omega_\nu(\hat{\mathbf{p}})$ and likewise of $Y_{lM}(\hat{\mathbf{p}})$,

$$(u, b_m\, u) \;=\; \sum_\nu \int_0^\infty dp\;\overline{a_\nu(p)} \int_0^\infty dp'\; b_{lsm}(p,p')\; a_\nu(p')$$

$$b_{lsm}(p,p') := \; b_{0m}(p)\;\delta(p-p') \;+\; b_{lsm}^{(1)}(p,p') \;+\; b_{lsm}^{(2)}(p,p') \tag{B.3}$$

where $b_{0m}(p) = E_p$,

$$b_{lsm}^{(1)}(p,p') \;=\; -\frac{\gamma}{\pi}\;\left[q_l(p/p') \;+\; h(p)\,h(p')\;q_{l+2s}(p/p')\right]\;A(p)\,A(p')$$

$$b_{lsm}^{(2)}(p,p') \;=\; \frac{1}{2}\;\left(\frac{\gamma}{\pi}\right)^2 \int_0^\infty dp''\;\left[\frac{1}{E_{p'}+E_{p''}} \;+\; \frac{1}{E_p+E_{p''}}\right]\;A(p)\,A(p')\;A^2(p'')$$

$$\cdot\,[q_l(p''/p)\;h(p'') \;-\; q_{l+2s}(p''/p)\;h(p)]\;[q_l(p''/p')\;h(p'') \;-\; q_{l+2s}(p''/p')\;h(p')]\,.$$

$A(p)$ and $h(p)$ are defined below (I.3.20). If $m = 0$, one has $E_p = p$ and $h(p) = 1$. On behalf of the symmetry $q_l(x) = q_l(1/x)$, the kernel reduces to the following form

$$b_0(p) \;=\; p$$

$$b_{ls}^{(1)}(p,p') \;=\; -\frac{\gamma}{2\pi}\;\left[q_l(p/p') + q_{l+2s}(p/p')\right] \tag{B.4}$$

$$b_{ls}^{(2)}(p,p') \;=\; \frac{\gamma^2}{8\pi^2} \int_0^\infty \frac{dp''}{p''}\;\left[q_l(p''/p) \;-\; q_{l+2s}(p''/p)\right]\;\left[q_l(p''/p') \;-\; q_{l+2s}(p''/p')\right].$$

From (B.4) it follows that $b_{ls}^{(1)}(p,p') \leq 0$ and $b_{ls}^{(2)}(p,p') \geq 0$ for all $p,p' \in \mathbb{R}_+$. This is a consequence of the property $0 \leq q_{l+1}(y) \leq q_l(y)$ for $y \neq 1$ and $l = 0,1,...$.

b) Mellin transform for $m = 0$

For a function $f \in L_2(\mathbb{R}_+)$ the Mellin transform $f^\#\in L_2(\mathbb{R})$, a unitary map, is defined by

$$f^\#(t) := \;\frac{1}{\sqrt{2\pi}} \int_0^\infty dp\; f(p)\; p^{-it-1/2}. \tag{B.5}$$

If $f \in \mathcal{S}(\mathbb{R}_+)$, it can be extended to an analytic function on the complex plane and satisfies for $\alpha \in \mathbb{C}$

$$(p^\alpha\, f)^\#(t) \;=\; f^\#(t+i\alpha). \tag{B.6}$$

Since the Mellin transform is unitary for $t \in \mathbb{R}$ (and for $p^\alpha f \in L_2(\mathbb{R}_+)$), the expectation value of the Jansen-Hess operator is invariant. Due to the scaling properties under dilations, the second-order kernel $b_{ls}^{(2)}(p,p')$ can be written in terms of a Mellin convolution, resulting in a factorisation of the two respective Mellin transforms. This leads to a kernel which can be cast into a diagonal form (Tix 1997, Stockmeyer 2002),

$$(u, b\,u) \;=\; \sum_\nu \int_{-\infty}^{\infty} dt\; \overline{a_\nu^\#(t)} \; \left(\int_0^\infty dp'\; b_{ls}(\cdot, p')\; a_\nu(p') \right)^\# (t) \tag{B.7}$$

$$= \sum_\nu \int_{-\infty}^{\infty} dt\; \overline{a_\nu^\#(t)}\; (b_0^\# \;+\; \sqrt{2\pi}\, b_{ls}^{(1)\#} \;+\; \sqrt{2\pi}\, b_{ls}^{(2)\#})(t)\; a_\nu^\#(t+i)$$

$$= \sum_\nu \int_{-\infty}^{\infty} dt\; \left| a_\nu^\#(t + \frac{i}{2}) \right|^2 \; \left(b_0^\# \;+\; \sqrt{2\pi}\, b_{ls}^{(1)\#} \;+\; \sqrt{2\pi}\, b_{ls}^{(2)\#} \right) (t - \frac{i}{2})$$

where the last equality results from a shift of the integration path by $-i/2$, made possible by the analyticity of the integrand, with

$$b_0^\#(t - \frac{i}{2}) \;=1, \qquad b_{ls}^{(1)\#}(t - \frac{i}{2}) \;=\; -\frac{\gamma}{2\pi} \left[q_l^\#(t - i/2) \;+\; q_{l+2s}^\#(t - i/2) \right]$$

$$b_{ls}^{(2)\#}(t - \frac{i}{2}) \;=\; \frac{\sqrt{2\pi}}{2} \left(\frac{\gamma}{2\pi} \right)^2 \left[q_l^\#(t - i/2) \;-\; q_{l+2s}^\#(t - i/2) \right]^2 . \tag{B.8}$$

The Mellin transformed reduced Legendre functions are defined in terms of the gamma function by

$$q_l^\#(t - \frac{i}{2}) \;=\; \frac{\sqrt{\pi}}{2\sqrt{2}} \, \frac{\Gamma(\frac{l}{2} + \frac{1}{2} - \frac{it}{2})}{\Gamma(\frac{l}{2} + 1 - \frac{it}{2})} \cdot \frac{\Gamma(\frac{l}{2} + \frac{1}{2} + \frac{it}{2})}{\Gamma(\frac{l}{2} + 1 + \frac{it}{2})}, \tag{B.9}$$

which are positive functions for real t. From this representation it follows that $b_{ls}^{(1)\#}(t - i/2) \;\leq 0$ and $b_{ls}^{(2)\#}(t - i/2) \;\geq 0$, and eventually $b \geq 0$ for subcritical potential strength γ.

Appendix C

Proof of the operator $|T|$-boundedness of the two-particle interactions for $m = 0$

a) Estimate of $\|V^{(12)}\,\psi\|$

In the one-particle case we have Hardy's inequality (see e.g. Herbst 1977)

$$(\varphi, \frac{e^4}{x^2}\,\varphi) \;\leq\; 4e^4\; (\varphi, p^2\,\varphi) \tag{C.1}$$

which can be derived from the Lieb and Yau formula (Lemma I.1), taking the convergence generating function $f(p) = p^{\frac{5}{2}}$. With this inequality we obtain

$$(\psi, (V^{(12)})^2\,\psi) \;=\; \int d\mathbf{x}_1\; d\mathbf{x}_2\; \overline{\psi(\mathbf{x}_1, \mathbf{x}_2)}\; \frac{e^4}{|\mathbf{x}_1 - \mathbf{x}_2|^2}\; \psi(\mathbf{x}_1, \mathbf{x}_2)$$

$$=\; e^4 \int d\mathbf{x}_1 \int d\mathbf{y}_2\; \overline{\varphi_{x_1}(\mathbf{y}_2)}\; \frac{1}{y_2^2}\; \varphi_{x_1}(\mathbf{y}_2) \;\leq\; 4e^4\; (\psi, p_2^2\,\psi) \tag{C.2}$$

where $\varphi_{x_1}(\mathbf{y}_2) := \psi(\mathbf{x}_1, \mathbf{y}_2 + \mathbf{x}_1)$ and the same strategy as in the proof of Lemma II.7 was used.

b) Estimate of $\|W^{(1)}\,\psi\|$

For the remaining parts of this appendix we use the unitary equivalence of the Sobolev transformed operators with the Douglas-Kroll transformed operators to work in the 2-spinor space, $u \in \mathcal{A}(H_1(\mathbb{R}^3) \times \mathbb{C}^2)^2$. As in the one-particle case, we make a partial wave decomposition of u with respect to the first variable,

$$\hat{u}(\mathbf{p}_1, \mathbf{p}_2) \;=\; \sum_{\nu \in I} p_1^{-1}\, a_{\nu,p_2}(p_1)\, \Omega_\nu(\hat{\mathbf{p}}_1), \qquad\qquad \nu = \{l, M, s\} \tag{C.3}$$

and keep in mind that the coefficient $a_{\nu,p_2}(p_1)$ depends additionally on $\mathbf{p}_2$. Then we can adopt the strategy of Mellin transform from Appendix B and obtain

$$(\psi, (W^{(1)})^2\, \psi) = ((b_{1m}+b_{2m})u, (b_{1m}+b_{2m})u) = (((b_{1m}+b_{2m})u)^{\#}, ((b_{1m}+b_{2m})u)^{\#})$$

$$= \int d\mathbf{p}_2 \sum_\nu \int_{-\infty}^{\infty} dt\; |a^{\#}_{\nu,p_2}(t+i)|^2\; (2\pi)\; |b^{(1)\#}_{ls}(t) \;+\; b^{(2)\#}_{ls}(t)|^2 \tag{C.4}$$

where b_{1m}, b_{2m} refer to particle 1 and $\#$ denotes Mellin transform with respect to p_1. The basic difference to the estimate of the *quadratic form* of $W^{(1)}$ is that the integrand of (C.4) is diagonal as it stands (and not only by a shift of coordinate t). Since $b^{(n)\#}_{ls}(t) \neq b^{(n)\#}_{ls}(t - \frac{i}{2}),\;\; n = 1, 2,$ new estimates for these complex functions have to be found. Using the explicit form (B.8) we have

$$|b^{(1)\#}_{ls}(t) \;+\; b^{(2)\#}_{ls}(t)|^2 \;\leq\; \Big(|b^{(1)\#}_{ls}(t)| \;+\; |b^{(2)\#}_{ls}(t)|\Big)^2 \tag{C.5}$$

$$= \left(\frac{\gamma}{2\pi}\; |q^{\#}_l(t) \;+\; q^{\#}_{l+2s}(t)| \;+\; \frac{\sqrt{2\pi}}{2} \left(\frac{\gamma}{2\pi}\right)^2\; |q^{\#}_l(t) \;-\; q^{\#}_{l+2s}(t)|^2\right)^2.$$

This expression is invariant under the transformation $(l, s) \;\mapsto\; (l + 2s, -s)$ and therefore we can restrict ourselves to $s = \frac{1}{2}$.

One can derive from (B.2) that $q_l'(y)$ is negative and $|q_l'(y)|$ is monotonically decreasing with l for $y > 1$ and $l \geq 0$. Therefore $0 \leq q_l(y) - q_{l+1}(y) \;\leq q_0(y) - q_1(y)$. From the definition (B.5) of the Mellin transform we obtain

$$|q^{\#}_l(t) \;\mp\; q^{\#}_{l+1}(t)| \;=\; \frac{1}{\sqrt{2\pi}} \left| \int_0^\infty dy\; (q_l(y) \;\mp\; q_{l+1}(y))\; y^{-it-\frac{1}{2}} \right|$$

$$\leq\; \frac{1}{\sqrt{2\pi}} \int_0^\infty \frac{dy}{\sqrt{y}}\; (q_0(y) \;\mp\; q_1(y)) \;=\; q^{\#}_0(0) \;\mp\; q^{\#}_1(0). \tag{C.6}$$

From the explicit representation of $q^{\#}_l(t - \frac{i}{2})$ for real t, (B.9), together with the identity theorem for complex $t = \frac{i}{2}$ and the functional equation $\Gamma(z+1) = z\Gamma(z)$, one gets

$$q^{\#}_l(0) \;=\; \frac{\sqrt{\pi}}{2\sqrt{2}}\, \frac{\Gamma(\frac{l+1}{2} + \frac{1}{4})\, \Gamma(\frac{l+1}{2} - \frac{1}{4})}{\Gamma(\frac{l}{2} + 1 + \frac{1}{4})\, \Gamma(\frac{l}{2} + 1 - \frac{1}{4})} \;=\; \frac{\sqrt{2\pi}}{2l+1} \tag{C.7}$$

such that

$$2\pi \left| b^{(1)\#}_{ls}(t) + b^{(2)\#}_{ls}(t) \right|^2 \leq 2\pi \left(\frac{\gamma}{2\pi}(\sqrt{2\pi} + \frac{\sqrt{2\pi}}{3}) + \frac{\sqrt{2\pi}}{2} \left(\frac{\gamma}{2\pi}\right)^2 (\sqrt{2\pi} - \frac{\sqrt{2\pi}}{3})^2 \right)^2$$

$$= \left(\frac{4}{3}\,\gamma \;+\; \frac{2}{9}\,\gamma^2\right)^2. \tag{C.8}$$

Since according to (B.6), $a^{\#}_{\nu,p_2}(t+i) \;=\; (p_1 a_{\nu,p_2}(p_1))^{\#}(t)$, we finally obtain

$$(\psi, (W^{(1)})^2\, \psi) \;\leq\; \int d\mathbf{p}_2 \sum_\nu \int_{-\infty}^{\infty} dt\; \left|(p_1\, a_{\nu,p_2}(p_1))^{\#}(t)\right|^2 \cdot \left(\frac{4}{3}\,\gamma \;+\; \frac{2}{9}\,\gamma^2\right)^2$$

$$= \left(\frac{4}{3}\,\gamma \;+\; \frac{2}{9}\,\gamma^2\right)^2\; (u, p_1^2\, u) \;=\; \left(\frac{4}{3}\,\gamma \;+\; \frac{2}{9}\,\gamma^2\right)^2\; (\psi, p_1^2\, \psi). \tag{C.9}$$

We remark that for the first-order contribution (linear in γ), we get $\|V^{(1)}\psi\| \le \tilde{c}\|p_1\psi\|$. The bound $\tilde{c} := \frac{4}{3}\gamma$ is sharp and considerably larger than the optimised bound $c = \frac{\gamma}{2}(\frac{\pi}{2} + \frac{2}{\pi}) = \gamma/\gamma_{BR}$ obtained from the quadratic form estimate $|(\psi, V^{(1)}\psi)| \le c\,(\psi, p_1\psi)$ according to Lemma II.6, viz. $\tilde{c}/c = 1.21$. This confirms that (positive) potentials with Coulomb-type singularities belong to the class A of operators for which the statement $(\psi, A\psi) \le c\,(\psi, p\,\psi) \implies (\psi, A^2\psi) \le c^2\,(\psi, p^2\psi)$ does *not* hold. (Another counter-example is the estimate of the Coulomb field with general wavefunctions (not restricted to the positive spectral subspace), compare Hardy's and Kato's inequality with a bound ratio of $4/\pi = 1.27$.)

c) Estimate of $|(\psi, W^{(1)}W^{(2)}\,\psi)|$

To this aim, we make a second partial wave decomposition of (C.3) with respect to the second variable $\mathbf{p}_2$,

$$\hat{u}(\mathbf{p}_1, \mathbf{p}_2) \;=\; \sum_{\nu\in I} p_1^{-1} \sum_{\nu'\in I} p_2^{-1}\, a_{\nu\nu'}(p_1,p_2)\, \Omega_\nu(\hat{\mathbf{p}}_1)\, \Omega_{\nu'}(\hat{\mathbf{p}}_2), \qquad \nu' = \{l'M's'\}. \tag{C.10}$$

It then follows that

$$(W^{(1)}\,\psi, W^{(2)}\,\psi) \;=\; \sum_{\nu\nu'} \int_0^\infty dp_1 \int_0^\infty dp_2\, \overline{\int_0^\infty dp_1'\; k_\nu(p_1,p_1')\; a_{\nu\nu'}(p_1',p_2)}$$
$$\cdot \int_0^\infty dp_2'\; k_{\nu'}(p_2,p_2')\; a_{\nu\nu'}(p_1,p_2') \tag{C.11}$$

where $k_\nu(p_1,p_1') := b_{lsm}^{(1)}(p_1,p_1') + b_{lsm}^{(2)}(p_1,p_1')$ is the kernel relating to $W^{(1)}$ and $k_{\nu'}(p_2,p_2')$ relates to $W^{(2)}$. The factorisation of the kernel of $W^{(1)}W^{(2)}$ allows for a factorisation of integrals in the generalised Lieb and Yau formula such that (with p_1 and p_1' interchanged)

$$|(W^{(1)}\,\psi, W^{(2)}\,\psi)| \;\le\; \sum_{\nu\nu'} \int_0^\infty dp_1 \int_0^\infty dp_2\; |a_{\nu\nu'}(p_1,p_2)|^2 \cdot I_\nu(p_1)\cdot I_{\nu'}(p_2)$$
$$I_\nu(p_1) := \int_0^\infty dp_1'\; |k_\nu(p_1',p_1)|\; \frac{f(p_1)}{f(p_1')} \tag{C.12}$$
$$I_{\nu'}(p_2) := \int_0^\infty dp_2'\; |k_{\nu'}(p_2,p_2')|\; \frac{g(p_2)}{g(p_2')}.$$

We can estimate $I_\nu(p_1)$ and $I_{\nu'}(p_2)$ as done in the proof of Proposition I.5 by functions which are independent of ν and ν'. Explicitly, starting from mass $m \neq 0$ and using (I.4.43) with (I.4.53),

$$I_\nu(p_1) \;\le\; \lim_{m\to 0} E_{p_1}\,(1 \,-\, \tilde{G}_{0\frac{1}{2}}(p_1/m)) \;\le\; p_1 \lim_{m\to 0}(1 \,-\, \inf_{p_1\in\mathbb{R}_+} \tilde{G}_{0\frac{1}{2}}(p_1/m))$$
$$=\; p_1\; \left[\frac{\gamma}{2}\left(\frac{\pi}{2} + \frac{2}{\pi}\right) \;+\; \frac{\gamma^2}{8}\left(\frac{\pi}{2} - \frac{2}{\pi}\right)^2\right] \tag{C.13}$$

where use has been made of the fact that $\inf\limits_{p_1\in\mathbb{R}_+} \tilde{G}_{0\frac{1}{2}}(p_1/m)$ is independent of m.

From this we get

$$|(\psi, W^{(1)}W^{(2)}\,\psi)| \;\le\; \left(\frac{\gamma}{2}\left(\frac{\pi}{2} + \frac{2}{\pi}\right) \;+\; \frac{\gamma^2}{8}\left(\frac{\pi}{2} - \frac{2}{\pi}\right)^2\right)^2\; (\psi, p_1 p_2\,\psi). \tag{C.14}$$

Appendix D

Proof of the norm convergence of the sequence $(W_{2n})_{n\in\mathbb{N}}$ of Hilbert-Schmidt operators for $m \neq 0$

As a typical example, we show first that $A_\epsilon := (T+\mu)^{-1}\, C_{1\epsilon}^{(12)}(e_\epsilon, f_\epsilon)\,(T+\mu)^{-1}$ has the property $|(\psi, A_\epsilon \psi)| \le c\cdot\epsilon$ and then that $B_\epsilon := (T+\mu)^{-1}\, R_{1\epsilon}^{(12)}(e_\epsilon, e_\epsilon)\,(T+\mu)^{-1}$ also is form bounded by some power of ϵ. $C_{1\epsilon}^{(12)}$ and $R_{1\epsilon}^{(1)}$ are defined in (II.6.14) – (II.6.16).

a) Estimate of A_ϵ

Using the generalised Lieb and Yau formula (II.3.7) with (II.3.8) we have

$$|(\psi, A_\epsilon\, \psi)| \;\le\; c_0 \int d\mathbf{p}_1\, d\mathbf{p}_2\, |\hat{\psi}(\mathbf{p}_1, \mathbf{p}_2)|^2\, (I_1 \,+\, I_2) \tag{D.1}$$

where I_1 and I_2 relate to the two parts of the kernel of A_ϵ. Estimating $|1 \pm \tilde{D}_0^{(1)}(\mathbf{p})| \le 2$, $(E_{p_1}+E_{p_2}+\mu)^{-1} \le (p_1+p_2+\mu)^{-1}$, $(E_{|\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1|}+E_{p_1'})^{-1} \le (|\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1|+m)^{-1}$, $(E_{p_1'}+E_{p_2'}+\mu)^{-1} \le (p_2'+\mu)^{-1}$ and setting the convergence generating functions $f = 1$ and $g(p) = p+1$, we obtain with the substitutions $\mathbf{q}_2 := \mathbf{p}_2' - \mathbf{p}_2$ for $\mathbf{p}_2'$ and $q_1 := \mathbf{p}_1' - \mathbf{p}_1 + \mathbf{p}_2' - \mathbf{p}_2$ for $\mathbf{p}_1'$,

$$I_1 \;\le c'\, \frac{1}{p_1+p_2+\mu}\, e^{-\epsilon(p_1+p_2)} \int d\mathbf{q}_1\, d\mathbf{q}_2\, \frac{1}{q_2^2+\epsilon^2}\, \frac{\epsilon^2}{q_1^2(q_1^2+\epsilon^2)}\, \frac{1}{|\mathbf{p}_1-\mathbf{q}_2|+m}$$
$$\cdot \frac{1}{|\mathbf{q}_2+\mathbf{p}_2|+\mu}\, \frac{p_2+1}{|\mathbf{q}_2+\mathbf{p}_2|+1}. \tag{D.2}$$

The $\mathbf{q}_1$-integral is according to (II.6.21) proportional to ϵ while the $\mathbf{q}_2$-integral is finite and independent of ϵ except for $m = 0$. In fact, setting $p_1 = m = 0$ and integrating near zero leads to a logarithmic ϵ dependence for $\epsilon \to 0$,

$$\int_0^1 q_2^2\, dq_2\, \frac{1}{q_2(q_2^2+\epsilon^2)} \;=\; \frac{1}{2}\int_{\epsilon^2}^{\epsilon^2+1} \frac{dz}{z} \;=\; \frac{1}{2}\left(\ln(1+\epsilon^2) \,-\, \ln\epsilon^2\right) \;\le\; \frac{1}{2}\ln 2 \,+\, |\ln\epsilon|. \tag{D.3}$$

Hence, $I_1 \le c_1\epsilon + c_2\epsilon\,|\ln\epsilon|$ with appropriate constants c_1 and c_2 independent of p_1 and p_2. If $m \neq 0$, the $\ln\epsilon$-term does not occur.

For the second integral I_2 we estimate $(E_{p_1}+E_{|\mathbf{p}_2'-\mathbf{p}_2+\mathbf{p}_1'|})^{-1} \le (m+|\mathbf{p}_2'-\mathbf{p}_2+\mathbf{p}_1'|)^{-1}$ and $e^{-\epsilon(p_1'+p_2')} \le 1$,

$$I_2 \;\le\; c'\, \frac{1}{p_1+p_2+\mu} \int d\mathbf{q}_1\, d\mathbf{q}_2\, \frac{1}{q_2^2+\epsilon^2}\, \frac{\epsilon^2}{q_1^2(q_1^2+\epsilon^2)}\, \frac{1}{m+|\mathbf{q}_1+\mathbf{p}_1|}$$
$$\cdot \frac{1}{|\mathbf{q}_2+\mathbf{p}_2|+\mu}\, \frac{p_2+1}{|\mathbf{q}_2+\mathbf{p}_2|+1}. \tag{D.4}$$

The $\mathbf{q}_2$-integral is finite and independent of ϵ for all p_2. This is trivial for $p_2 = 0$ whereas for large p_2 (with $\frac{p_2+1}{p_1+p_2+\mu} \le 1$ and Appendix A)

$$\int d\mathbf{q}_2\, \frac{1}{q_2^2+\epsilon^2}\, \frac{1}{|\mathbf{q}_2+\mathbf{p}_2|+\mu}\, \frac{1}{|\mathbf{q}_2+\mathbf{p}_2|+1} \;\le\; \int d\mathbf{q}_2\, \frac{1}{q_2^2}\, \frac{1}{|\mathbf{q}_2+\mathbf{p}_2|^2} \;=\; \frac{\pi^3}{p_2}. \tag{D.5}$$

The q_1-integral is pathological for $p_1 = 0$ when m tends to zero. In fact,

$$\int_0^\infty dq_1\, \frac{\epsilon^2}{q_1^2+\epsilon^2}\, \frac{1}{q_1+m} \;=\; \lim_{R\to\infty} \frac{\epsilon^2}{m^2+\epsilon^2} \int_0^R dq_1 \left(\frac{-q_1+m}{q_1^2+\epsilon^2} \;+\; \frac{1}{q_1+m}\right)$$
$$=\; \frac{m\epsilon}{m^2+\epsilon^2}\left(\frac{\epsilon}{m}\,\ln\frac{\epsilon}{m} \,+\, \frac{\pi}{2}\right) \;\le\; c_1\epsilon \,+\, c_2\epsilon^2\ln\epsilon \,+\, O(\epsilon^2), \qquad (m \neq 0). \tag{D.6}$$

The integral (D.6) diverges logarithmically with m for fixed ϵ as $m \to 0$, and tends to $\frac{\pi}{4}$ if $m = \epsilon = \frac{1}{n} \to 0$. Thus I_2 is no longer bounded by ϵ for all p_1, p_2 when $m \to 0$. In order to include the massless case in the proof, a more careful decomposition should replace (II.6.15).

Collecting results

$$|(\psi, A_\epsilon\, \psi)| \;\le\; \epsilon\, \|\psi\|^2\; (c \,+\, C\,\epsilon \ln \epsilon \,+\, O(\epsilon))$$
$$\longrightarrow\; 0 \qquad\qquad (\epsilon \to 0, \quad m \ne 0) \tag{D.7}$$

with suitable constants c, C.

In a similar way, the operator involving $C_{1\epsilon}^{(12)}(f_\epsilon, e_\epsilon)$ can be estimated by the r.h.s. of (D.7), while the third term, $C_{1\epsilon}^{(12)}(f_\epsilon, f_\epsilon)$, leads to an estimate which vanishes to higher order in ϵ.

b) Estimate of B_ϵ

We start from

$$|(\psi, B_\epsilon\, \psi)| \;\le\; c_0' \int d\mathbf{p}_1\, d\mathbf{p}_2\, |\hat{\psi}(\mathbf{p}_1, \mathbf{p}_2)|^2\, (J_1 \,+\, J_2) \tag{D.8}$$

and choose the convergence generating functions $f(p) = p$ and $g = 1$. Then one estimates the integral J_1 corresponding to the first part of the kernel of B_ϵ by

$$J_1 \;\le\; c'\, \frac{1}{p_1 + p_2 + \mu} \left(1 \,-\, e^{-\epsilon(p_1+p_2)}\right) \int d\mathbf{p}_1'\, d\mathbf{p}_2'\, \frac{1}{|\mathbf{p}_2 - \mathbf{p}_2'|^2 + \epsilon^2}$$
$$\cdot \frac{1}{|\mathbf{p}_2 - \mathbf{p}_2' + \mathbf{p}_1 - \mathbf{p}_1'|^2 + \epsilon^2}\; \frac{1}{E_{|\mathbf{p}_2 - \mathbf{p}_2' + \mathbf{p}_1|} + E_{p_1'}}\; \frac{1}{p_1' + p_2' + \mu}\; \frac{p_1}{p_1'}. \tag{D.9}$$

When (D.9) is estimated by setting $\epsilon = 0$ in the two denominators and when $(p_1' + p_2' + \mu)^{-1} \le 1/p_1'$ is used, the integral coincides with one given in the proof of Lemma II.4. From (II.5.5) to (II.5.8), together with the estimate ϵ of the prefactor according to (II.6.22) one finds

$$J_1 \;\le\; c'\, \epsilon \cdot \pi^6/2. \tag{D.10}$$

For the second integral J_2 we estimate by setting $\epsilon = 0$ as before and make the substitutions $\mathbf{q}_2 := \mathbf{p}_2' - \mathbf{p}_2$ for $\mathbf{p}_2'$ and $\mathbf{q}_1 := \mathbf{q}_2 + \mathbf{p}_1'$ for $\mathbf{p}_1'$. Then

$$J_2 \;\le\; c'\, \frac{1}{p_1 + p_2 + \mu} \int d\mathbf{q}_1\, d\mathbf{q}_2\, \frac{1}{q_2^2}\, \frac{1}{|\mathbf{q}_1 - \mathbf{p}_1|^2}\, \frac{1}{E_{p_1} + E_{q_1}} \tag{D.11}$$
$$\cdot \left[\left(1 \,-\, e^{-\epsilon(p_1' + p_2')}\right)\, \frac{1}{p_1' + p_2' + \mu}\right]\, \frac{p_1}{p_1'}.$$

In this expression, we can no longer use the estimate (II.6.22) for the term in square brackets because the remaining integral does not converge. Rather, we consider the factor $1 - e^{-\epsilon p}$ with $p := p_1' + p_2' = |\mathbf{q}_1 - \mathbf{q}_2| + |\mathbf{q}_2 + \mathbf{p}_2|$ as a function of $x := \epsilon^{\frac{1}{2}}$. Then its derivative is

$$\frac{d}{dx}\, f(x) := \frac{d}{dx}\, \left(1 \,-\, e^{-x^2 p}\right) \;=\; 2xp\, e^{-x^2 p} \;\ge\; 0 \tag{D.12}$$

with its maximum given by $\max\limits_{x \ge 0} (2xp\, e^{-x^2 p}) \;=\; \sqrt{2p}\, e^{-\frac{1}{2}}$. Accordingly, one can Taylor expand,

$$f(x) \;=\; f(0) \,+ x\, \frac{d}{dx}\, f(x)\Big|_{x=0} \;+\; O(x^2). \tag{D.13}$$

Since $f(0) = 0$, one has from the mean value theorem the estimate $|f(x)| \le x \cdot \sqrt{2p}\, e^{-\frac{1}{2}}$, and the integral corresponding to the linear term in x provides a convergent majorant:

$$M := \int d\mathbf{q}_1\, d\mathbf{q}_2\, \frac{1}{q_2^2}\, \frac{1}{|\mathbf{q}_1 - \mathbf{p}_1|^2}\, \frac{1}{E_{p_1} + E_{q_1}}\, \frac{\sqrt{p_1' + p_2'}}{p_1' + p_2' + \mu}\, \frac{1}{p_1'}. \tag{D.14}$$

Estimating $(E_{p_1} + E_{q_1})^{-1} \le 1/q_1$ and $\dfrac{\sqrt{p_1' + p_2'}}{p_1' + p_2' + \mu} \le \dfrac{1}{\sqrt{p_1' + p_2'}} \le \dfrac{1}{p_1'^{\frac{1}{2}}}$ one has

$$M \;\le\; \int \frac{d\mathbf{q}_1}{q_1}\, \frac{1}{|\mathbf{q}_1 - \mathbf{p}_1|^2} \int \frac{d\mathbf{q}_2}{q_2^2}\, \frac{1}{|\mathbf{q}_1 - \mathbf{q}_2|^{\frac{3}{2}}}. \tag{D.15}$$

With the substitution $\mathbf{p} := \mathbf{q}_2 - \mathbf{q}_1$, the second integral can be estimated with the help of Appendix A,

$$\int \frac{d\mathbf{p}}{p^{\frac{3}{2}}}\, \frac{1}{|\mathbf{p} + \mathbf{q}_1|^2} \;=\; \frac{2\pi}{q_1} \int_0^\infty \frac{dp}{\sqrt{p}}\, \ln \frac{p + q_1}{|p - q_1|} \;=\; \frac{2\pi}{\sqrt{q_1}} \int_0^\infty \frac{dy}{\sqrt{y}}\, \ln \frac{y+1}{|y-1|} \;=\; \frac{(2\pi)^2}{\sqrt{q_1}}. \tag{D.16}$$

The remaining integral is the same as (D.16) such that $M \le \dfrac{\text{const}}{\sqrt{p_1}}$. Insertion into (D.11) gives

$$J_2 \;\le\; c'\, \frac{1}{p_1 + p_2 + \mu}\, M\, x\sqrt{2}\, e^{-\frac{1}{2}} \cdot p_1 \;\le\; c\,\sqrt{\epsilon} \tag{D.17}$$

with c a suitable constant independent of p_1 and p_2.

c) Estimate of remaining terms

In the remaining three contributions to $W_2 - W_{2n}$ which contain the factors $R_{1\epsilon}^{(12)}(e_\epsilon, f_\epsilon)$, $R_{1\epsilon}^{(12)}(f_\epsilon, e_\epsilon)$ and $R_{1\epsilon}^{(12)}(f_\epsilon, f_\epsilon)$, the following estimate can be made,

$$\frac{\epsilon^2}{p^2(p^2 + \epsilon^2)} \;\le\; \frac{\epsilon^2}{p^2 \cdot \epsilon^2} \;\le\; \frac{1}{p^2}, \tag{D.18}$$

which reduces them exactly to the estimate of the operator B_ϵ after the additional ϵ^2 in the denominators have been dropped.

Collecting results, we have proved that in lowest order of ϵ,

$$|(\psi, (T + \mu)^{-1}\, \left(C_1^{(12)} \;-\; C_{1\epsilon}^{(12)}(e_\epsilon, e_\epsilon)\right)\, (T + \mu)^{-1}\, \psi)\,| \;\le\; c\, \epsilon^{\frac{1}{2}}\, \|\psi\|^2. \tag{D.19}$$

The operator boundedness follows from (D.19) by means of Lemma I.3.

Appendix E

Estimate of the Jansen-Hess term B_{2m} in coordinate space

Our goal is to show boundedness of the integral in (I.4.24), $\int d\mathbf{x}'\, |k(\mathbf{x}, \mathbf{x}')|\, \frac{f(x)}{f(x')}$, relative to the Coulomb field γ/x, for arbitrary mass $m \ge 0$.

We take $f(x) = x$ and obtain with (I.4.23) and (I.3.27) for the kernel k of B_{2m},

$$k(\mathbf{x}, \mathbf{x}') \;=\; c_0 \int d\mathbf{p}\, e^{i\mathbf{p}\mathbf{x}} \int d\mathbf{p}'\, e^{-i\mathbf{p}'\mathbf{x}'} \int d\mathbf{p}''\, \frac{1}{|\mathbf{p}'' - \mathbf{p}|^2}\, \frac{1}{|\mathbf{p}'' - \mathbf{p}'|^2}$$
$$\cdot (1 \;-\; \tilde{D}_0(\mathbf{p}''))\, \left(\frac{1}{E_{p''} + E_p} \;+\; \frac{1}{E_{p''} + E_{p'}}\right) \tag{E.1}$$

with $c_0 := \frac{1}{(2\pi)^3}\,\frac{\gamma^2}{16\pi^4}$. We recall the Coulombic integrals,

$$\int d\mathbf{q}\; e^{i\mathbf{q}\mathbf{x}}\;\frac{1}{q^2} \;=\; \frac{2\pi^2}{x}$$

$$\int d\mathbf{q}\; e^{i\mathbf{q}\mathbf{x}}\;\frac{1}{q} \;=\; \frac{4\pi}{x^2} \tag{E.2}$$

and use the first one for the $\mathbf{p}'$-integral (with the variable shift $\mathbf{q}' := \mathbf{p}' - \mathbf{p}''$) respective $\mathbf{p}$-integral to obtain

$$k(\mathbf{x},\mathbf{x}') \;=\; 2\pi^2 c_0\, \left(\frac{1}{x'}\,I_1 \;+\; \frac{1}{x}\,I_2\right), \tag{E.3}$$

$$I_1 := \int d\mathbf{p}\; d\mathbf{p}''\; e^{i\mathbf{p}\mathbf{x}}\; e^{-\mathbf{p}''\mathbf{x}'}\;\frac{1}{|\mathbf{p}''-\mathbf{p}|^2}\;(1\,-\,\tilde{D}_0(\mathbf{p}''))\;\frac{1}{E_{p''}+E_p}$$

$$I_2 := \int d\mathbf{p}'\; d\mathbf{p}''\; e^{i\mathbf{p}''\mathbf{x}}\; e^{-i\mathbf{p}'\mathbf{x}'}\;\frac{1}{|\mathbf{p}''-\mathbf{p}'|^2}\;(1\,-\,\tilde{D}_0(\mathbf{p}''))\;\frac{1}{E_{p''}+E_{p'}}.$$

We make the substitutions $\mathbf{q} := \mathbf{p}'' - \mathbf{p}$ and $\mathbf{q} := \mathbf{p}'' - \mathbf{p}'$ for $\mathbf{p}$ and $\mathbf{p}'$ in I_1 and I_2, respectively. This turns the energy denominators into $(E_{p''} + E_{|\mathbf{p}''-\mathbf{q}|})^{-1}$, and additionally one gets the factor $\frac{1}{q^2}$.

Since $\|1 - \tilde{D}_0(\mathbf{p}'')\| = 2$, the symbol class of B_{2m} is not changed if $1 - \tilde{D}_0(\mathbf{p}'')$ is replaced by 2. Also, it is not changed if in the energy denominators, one sets $q = 0$ and drops the mass. Then k is estimated by

$$|k(\mathbf{x},\mathbf{x}')| \;\le\; C\cdot 2\pi^2 c_0\, \left\{\frac{1}{x'}\,\left(\int d\mathbf{q}\; e^{-i\mathbf{q}\mathbf{x}}\;\frac{1}{q^2}\right)\,\left(\int d\mathbf{p}''\; e^{i\mathbf{p}''(\mathbf{x}-\mathbf{x}')}\;\frac{1}{p''}\right)\right.$$

$$\left. +\,\frac{1}{x}\,\left(\int d\mathbf{q}\; e^{i\mathbf{q}\mathbf{x}'}\;\frac{1}{q^2}\right)\,\left(\int d\mathbf{p}''\; e^{i\mathbf{p}''(\mathbf{x}-\mathbf{x}')}\;\frac{1}{p''}\right)\right\}$$

$$=\; C\cdot 4\pi^2 c_0\;\frac{1}{x'}\cdot\frac{2\pi^2}{x}\cdot\frac{4\pi}{|\mathbf{x}-\mathbf{x}'|^2} \tag{E.4}$$

with some constant C, using that both terms, resulting from I_1/x' and I_2/x, are equal. Integration over $\mathbf{x}'$ leads with the help of Appendix A to

$$\int d\mathbf{x}'\;|k(\mathbf{x},\mathbf{x}')|\;\frac{f(x)}{f(x')} \;\le\; C\cdot\frac{\gamma^2}{4\pi^2}\;\frac{1}{x}\;\int d\mathbf{x}'\;\frac{1}{x'}\;\frac{1}{|\mathbf{x}-\mathbf{x}'|^2}\cdot\frac{x}{x'}$$

$$=\; C\cdot\frac{\pi}{4}\,\gamma^2\;\frac{1}{x}. \tag{E.5}$$

Appendix F

Estimate of the second-order two-particle potential $C^{(12)}$ in coordinate space

We want to prove boundedness of the integral in (II.5.30), $\frac{1}{(2\pi)^6}\int\, d\mathbf{x}_1' d\mathbf{x}_2'\,|k(\mathbf{x}_1,\mathbf{x}_2;\mathbf{x}_1',\mathbf{x}_2')|\,\frac{f(x_1)}{f(x_1')}\,\frac{g(x_2)}{g(x_2')}$ relative to the electron-electron potential $\frac{e^2}{|\mathbf{x}_1-\mathbf{x}_2|}$.

We choose $f(x) = x^2$ and $g = 1$. For the kernel k of $C^{(12)}$ we have from (II.5.29) and (II.4.10),

$$k(\mathbf{x}_1,\mathbf{x}_2;\mathbf{x}_1',\mathbf{x}_2') \;=\; c_1\int d\mathbf{p}_1\, d\mathbf{p}_2\, d\mathbf{p}_1'\, d\mathbf{p}_2'\; e^{i\mathbf{p}_1\mathbf{x}_1}\; e^{i\mathbf{p}_2\mathbf{x}_2}\;\frac{1}{|\mathbf{p}_2-\mathbf{p}_2'|^2} \tag{F.1}$$

$$\cdot \frac{1}{|\mathbf{p}_2 - \mathbf{p}_2' + \mathbf{p}_1 - \mathbf{p}_1'|^2} \left\{ \frac{1}{E_{|\mathbf{p}_2-\mathbf{p}_2'+\mathbf{p}_1|} + E_{p_1'}} \, (1 - \tilde{D}_0^{(1)}(\mathbf{p}_2 - \mathbf{p}_2' + \mathbf{p}_1)) \, (1 + \tilde{D}_0^{(1)}(\mathbf{p}_1')) \right.$$

$$\left. + \frac{1}{E_{p_1} + E_{|\mathbf{p}_2'-\mathbf{p}_2+\mathbf{p}_1'|}} \, (1 + \tilde{D}_0^{(1)}(\mathbf{p}_1)) \, (1 - \tilde{D}_0^{(1)}(\mathbf{p}_2' - \mathbf{p}_2 + \mathbf{p}_1')) \right\} e^{-i\mathbf{p}_1'\mathbf{x}_1'} \, e^{-i\mathbf{p}_2'\mathbf{x}_2'}$$

with $c_1 := -\frac{2\gamma e^2}{(2\pi)^4}$. We make the substitutions $\mathbf{q}_2 := \mathbf{p}_2 - \mathbf{p}_2'$ for $\mathbf{p}_2$ and $\mathbf{q}_1 := \mathbf{p}_2 - \mathbf{p}_2' + \mathbf{p}_1 - \mathbf{p}_1'$ for $\mathbf{p}_1$ such that the remaining integration over $\mathbf{p}_2'$ becomes trivial. Then,

$$k(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}_1', \mathbf{x}_2') \;=\; (2\pi)^3 c_1 \, \delta(\mathbf{x}_2 - \mathbf{x}_2') \left(\int d\mathbf{q}_2 \, e^{i\mathbf{q}_2(\mathbf{x}_2 - \mathbf{x}_1)} \, \frac{1}{q_2^2} \right)$$

$$\cdot \int d\mathbf{q}_1 \, d\mathbf{p}_1' \, e^{i\mathbf{q}_1\mathbf{x}_1} \, \frac{1}{q_1^2} \, e^{i\mathbf{p}_1'(\mathbf{x}_1 - \mathbf{x}_1')} \, (I_1 \,+\, I_2)$$

$$I_1 := \frac{1}{E_{|\mathbf{q}_1+\mathbf{p}_1'|} + E_{p_1'}} \, (1 - \tilde{D}_0^{(1)}(\mathbf{q}_1 + \mathbf{p}_1')) \, (1 + \tilde{D}_0^{(1)}(\mathbf{p}_1')) \tag{F.2}$$

$$I_2 := \frac{1}{E_{|\mathbf{q}_1-\mathbf{q}_2+\mathbf{p}_1'|} + E_{|\mathbf{p}_1'-\mathbf{q}_2|}} \, (1 + \tilde{D}_0^{(1)}(\mathbf{q}_1 - \mathbf{q}_2 + \mathbf{p}_1')) \, (1 - \tilde{D}_0^{(1)}(\mathbf{p}_1' - \mathbf{q}_2)).$$

The integral in brackets is evaluated by means of (E.2). Since $\|1 \pm \tilde{D}_0^{(1)}\| = 2$, the symbol class of $C^{(12)}$ is not changed upon replacing $(1-\tilde{D}_0^{(1)}(\mathbf{q}_1+\mathbf{p}_1'))(1+\tilde{D}_0^{(1)}(\mathbf{p}_1'))$ by 4 in I_1 and similarly in I_2. Note, however, that this is a rather crude estimate.

Moreover, we can replace $\mathbf{q}_1$ and $\mathbf{q}_2$ in the energy denominators of I_1 and I_2 by zero, and also set $m = 0$, without changing the symbol class of $C^{(12)}$. This is a good estimate since, due to the factors q_1^{-2} and q_2^{-2}, small values of q_1 and q_2 give an essential contribution to the integrals. We conjecture that the constant C, picked up by these estimates, should be $\frac{1}{2} \lesssim C \lesssim 1$. We get

$$|k(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}_1', \mathbf{x}_2')| \;\leq\; (2\pi)^3 \, |c_1| \, 4 \, C \, \delta(\mathbf{x}_2 - \mathbf{x}_2') \, \frac{2\pi^2}{|\mathbf{x}_2 - \mathbf{x}_1|}$$

$$\cdot \, 2 \left(\int d\mathbf{q}_1 \, e^{i\mathbf{q}_1\mathbf{x}_1} \, \frac{1}{q_1^2} \right) \left(\int d\mathbf{p}_1' \, e^{i\mathbf{p}_1'(\mathbf{x}_1 - \mathbf{x}_1')} \, \frac{1}{2p_1'} \right)$$

$$= \; (2\pi)^6 \cdot 8\pi^2 \, |c_1| \, C \, \delta(\mathbf{x}_2 - \mathbf{x}_2') \, \frac{1}{|\mathbf{x}_2 - \mathbf{x}_1|} \, \frac{1}{x_1} \, \frac{1}{|\mathbf{x}_1 - \mathbf{x}_1'|^2} \tag{F.3}$$

where again (E.2) was used.

With the help of Appendix A, the integration over $\mathbf{x}_1', \mathbf{x}_2'$ leads to

$$\frac{1}{(2\pi)^6} \int d\mathbf{x}_1' \, d\mathbf{x}_2' \, |k(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}_1', \mathbf{x}_2')| \, \frac{f(x_1)}{f(x_1')} \cdot \frac{g(x_2)}{g(x_2')} \tag{F.4}$$

$$= \; 8\pi^2 \, |c_1| \, C \, \frac{1}{|\mathbf{x}_2 - \mathbf{x}_1|} \int d\mathbf{x}_1' \, \frac{1}{|\mathbf{x}_1 - \mathbf{x}_1'|^2} \cdot \frac{x_1}{x_1'^2} \;=\; C \, \pi\gamma \, \frac{e^2}{|\mathbf{x}_2 - \mathbf{x}_1|}.$$

Appendix G

On the relation of the kernels $b_{lsm}^{(2)}(p,p')$ and $b_{lsm}^{(1)}(p,p')$ of the Jansen-Hess operator

In the massless case, we know from Proposition I.3 that $-b_1 \geq b_2 \geq 0$ for subcritical γ. We will show that this inequality does not hold for the respective kernels of b_1 and b_2, i.e. there exist $p, p' \in \mathbb{R}_+$ such that $b_{ls}^{(2)}(p,p') \geq -b_{ls}^{(1)}(p,p')$.

We start by restricting ourselves to the ground state ($l=0, s=\frac{1}{2}$) and define for $m=0$

$$f_1(p,p') := \; q_0(p/p') \,+\, q_1(p/p') \tag{G.1}$$

$$f_2(p,p') := \int_0^\infty \frac{dp''}{p''} \left[q_0(\frac{p''}{p}) \,-\, q_1(\frac{p''}{p}) \right] \left[q_0(\frac{p''}{p'}) \,-\, q_1(\frac{p''}{p'}) \right]$$

such that $-b_1(p,p') \geq b_2(p,p') \iff f_1(p,p') \geq \frac{\gamma}{4\pi} f_2(p,p')$ according to (B.4).

First we note that the above inequality holds for $p=p'\neq 0$ since $q_0(p/p') = \ln \frac{p+p'}{|p-p'|}$, and hence $f_1(p,p')$ diverges logarithmically. On the other hand, $f_2(p,p')$ remains finite for $p\neq 0$,

$$f_2(p,p) \;=\; \int_0^\infty \frac{dp''}{p''} \left(q_0(\frac{p''}{p}) \,-\, q_1(\frac{p''}{p}) \right)^2 \;<\; \infty \tag{G.2}$$

since

$$q_0(y) \;=\; q_0(1/y) \;=\; 2y \,+\, \frac{2}{3}\,y^3 \,+\, O(y^5) \tag{G.3}$$

$$q_1(y) \;=\; q_1(1/y) \;=\; \frac{4}{3}\,y^2 \,+\, O(y^4) \qquad\qquad \text{for } y\to 0.$$

Let us now for fixed $p\in\mathbb{R}_+$ consider the behaviour when p' tends to infinity. Then from (G.3),

$$f_1(p,p') \;=\; \frac{2p}{p'} \,+\, O(\frac{p}{p'})^2. \tag{G.4}$$

We will show that $f_2(p,p')$ behaves like $\frac{\ln p'}{p'}$ for large p'. Since $q_0(y) > q_1(y)$ for small $y\neq 0$ (see (G.3)), we need only consider q_0 in the second square bracket of (G.1). We split the remaining integral into two parts,

$$I_1 := \int_0^1 \frac{dp''}{p''} \left(q_0(\frac{p''}{p}) \,-\, q_1(\frac{p''}{p}) \right) \, q_0(\frac{p''}{p'})$$

$$I_2 := \int_1^\infty \frac{dp''}{p''} \left(q_0(\frac{p''}{p}) \,-\, q_1(\frac{p''}{p}) \right) \, q_0(\frac{p''}{p'}). \tag{G.5}$$

Recalling that $q_0(p''/p') \sim \frac{p''}{p'}$ for $p'\to\infty$, and $q_0(p''/p) \sim \frac{p}{p''}$ for $p''\to\infty$, it is obvious that I_2 decreases weaker with p' than $\sim \frac{1}{p'}$. To make this more explicit, we subtract and add the asymptotic behaviour of $q_0(p''/p)$,

$$I_2 \;=\; I_{21} \,+\, I_{22}, \tag{G.6}$$

$$I_{21} := \int_1^\infty \frac{dp''}{p''} \left(q_0(\frac{p''}{p}) \,-\, q_1(\frac{p''}{p}) \,-\, \frac{2p}{p''} \right) \, q_0(\frac{p''}{p'})$$

$$I_{22} := \; 2p \int_1^\infty \frac{dp''}{p''^2} \, q_0(\frac{p''}{p'}).$$

From (G.3), the integrand of I_{21} behaves $\sim \frac{1}{p''} \left(\frac{2}{3}\frac{p^3}{p''^3} - \frac{4}{3}\frac{p^2}{p''^2} \right) \cdot \frac{p''}{p'}$ for $p'\to\infty$ and p'' large, such that the p''-integral is convergent at the upper limit, giving $I_{21} \sim \frac{cp}{p'}$ for $p'\to\infty$.

The integral I_{22} can be evaluated analytically. Let $x := 1/p''$, such that with $q := 1/p'$,

$$I_{22} \;=\; 2p \int_0^1 dx \; \ln \frac{x+1/p'}{|x-1/p'|} \;=\; 2p \int_0^1 dx \; \left(\ln(x+q) \,-\, \ln|x-q| \right) \tag{G.7}$$

$$=\; 2p \left[(1+q)\ln(1+q) \,-\, 2q\ln q \,-\, (1-q)\ln(1-q) \right] \;\longrightarrow\; 2p\,(-2q\ln q) \;=\; 4p\,\frac{\ln p'}{p'}$$

for $q\to 0$, i.e. $p'\to\infty$. It remains to show that $I_1 \sim \frac{1}{p'}$ for $p'\to\infty$ such that the logarithmic singularity is not cancelled. But this is trivial since the integrand of I_1

is finite both on the upper and lower integration limit (or in case of $p'' = p = 1$ it has an integrable singularity). This proves that

$$f_2(p,p') \sim \frac{c\,p\,\ln p'}{p'} \qquad \text{for } p' \to \infty \tag{G.8}$$

such that $\frac{\gamma}{4\pi} f_2(p,p') > f_1(p,p')$ for arbitrary $\gamma > 0$ and sufficiently large p'.

It can easily be shown from the behaviour of $q_l(p''/p')$ for higher l that

$$\frac{b^{(2)}_{ls}(p,p')}{-b^{(1)}_{ls}(p,p')} \sim c\,\ln p' \qquad \text{for } p' \to \infty \tag{G.9}$$

holds also for $l > 0$.

We remark that a numerical calculation reproduces this singular behaviour for $m = 1$, such that due to the scaling property (I.4.35) it holds true for all m.

Appendix H

Estimate of the second-order contribution to the virial theorem for b_m

The operator T_2 defined in (I.5.26) is given explicitly by

$$T_2(\mathbf{p},\mathbf{p}') := \int d\mathbf{p}''\, \frac{1}{|\mathbf{p}-\mathbf{p}''|^2}\, \frac{1}{|\mathbf{p}''-\mathbf{p}'|^2} \tag{H.1}$$

$$\Bigg\{ -\frac{p''^2}{2E_{p''}(E_{p''}+m)} \left[\frac{m}{E_{p''}} \left(\frac{1}{E_{p'}}\frac{1}{E_{p'}+E_{p''}} + \frac{1}{E_p}\frac{1}{E_p+E_{p''}} \right) + \left(\frac{1}{E_{p'}+E_{p''}} + \frac{1}{E_p+E_{p''}} \right) \left(\frac{1}{E_{p''}} + \frac{m}{E_{p''}^2} \right) \right]$$

$$+ \boldsymbol{\sigma}\hat{\mathbf{p}}''\,\boldsymbol{\sigma}\hat{\mathbf{p}}'\, \frac{p'p''}{2E_{p''}(E_{p'}+m)} \left[\frac{m}{E_{p''}} \left(\frac{1}{E_{p'}}\frac{1}{E_{p'}+E_{p''}} + \frac{1}{E_p}\frac{1}{E_p+E_{p''}} \right) + \left(\frac{1}{E_{p'}+E_{p''}} + \frac{1}{E_p+E_{p''}} \right) \left(\frac{1}{E_{p'}} + \frac{m}{E_{p''}^2} \right) \right]$$

$$+ \boldsymbol{\sigma}\hat{\mathbf{p}}''\,\boldsymbol{\sigma}\hat{\mathbf{p}}\, \frac{pp''}{2E_{p''}(E_p+m)} \left[\frac{m}{E_{p''}} \left(\frac{1}{E_{p'}(E_{p'}+E_{p''})} + \frac{1}{E_p(E_p+E_{p''})} \right) + \left(\frac{1}{E_{p'}+E_{p''}} + \frac{1}{E_p+E_{p''}} \right) \left(\frac{1}{E_p} + \frac{m}{E_{p''}^2} \right) \right]$$

$$- \boldsymbol{\sigma}\hat{\mathbf{p}}\,\boldsymbol{\sigma}\hat{\mathbf{p}}'\, \frac{pp'(E_{p''}+m)}{2E_{p''}(E_p+m)(E_{p'}+m)} \left[\frac{m}{E_{p''}} \left(\frac{1}{E_{p'}}\frac{1}{E_{p'}+E_{p''}} + \frac{1}{E_p}\frac{1}{E_p+E_{p''}} \right) + \left(\frac{1}{E_{p'}+E_{p''}} + \frac{1}{E_p+E_{p''}} \right) \left(\frac{1}{E_p} + \frac{1}{E_{p'}} - \frac{1}{E_{p''}} + \frac{m}{E_{p''}^2} \right) \right] \Bigg\}.$$

We demonstrate the procedure of estimating the integral over $T_2(\mathbf{p},\mathbf{p}')$ introduced in (I.5.27) for one particular term,

$$I := \int d\mathbf{p}'d\mathbf{p}''\, |\boldsymbol{\sigma}\hat{\mathbf{p}}''\,\boldsymbol{\sigma}\hat{\mathbf{p}}'|\, \frac{p'p''}{2E_{p''}(E_{p'}+m)}\, \frac{m}{E_{p''}E_p}\, \frac{1}{E_p+E_{p''}} \cdot \frac{1}{|\mathbf{p}-\mathbf{p}''|^2}\, \frac{1}{|\mathbf{p}''-\mathbf{p}'|^2}\, \frac{f(p)}{f(p')}. \tag{H.2}$$

We take $f(p) := p^{5/2}/(E_p+m)$ and make the substitutions $\mathbf{q}'' := \dfrac{\mathbf{p}''}{mq}$ and $\mathbf{q}' := \dfrac{\mathbf{p}'}{mqq''}$ for $\mathbf{p}''$ and $\mathbf{p}'$, respectively. We estimate $|\boldsymbol{\sigma}\hat{\mathbf{p}}''\,\boldsymbol{\sigma}\hat{\mathbf{p}}'|$ by 1 and set $\mathbf{q} := \mathbf{p}/m$. Then the angular integrations can be performed with the help of (A.1), such that

$$I \;\leq\; 2\pi^2 q^4\,\frac{1}{\sqrt{q^2+1}}\,\frac{1}{\sqrt{q^2+1}+1}\int_0^\infty dq'\,\frac{1}{q'^{\frac{1}{2}}}\,\ln\left|\frac{1+q'}{1-q'}\right|$$

$$\cdot\int_0^\infty dq''q''^{\frac{3}{2}}\,\ln\left|\frac{1+q''}{1-q''}\right|\,\frac{1}{(qq'')^2+1}\,\frac{1}{\sqrt{q^2+1}+\sqrt{(qq'')^2+1}} \tag{H.3}$$

We estimate the last factor with the help of $\sqrt{(qq'')^2+1}\;\geq 1$ and then use the estimate (I.5.28) to obtain

$$I \;\leq\; 4\pi^3 q^4\,\frac{1}{\sqrt{q^2+1}}\,\frac{1}{(\sqrt{q^2+1}+1)^2}\left[\int_0^{1/q} dq''q''^{\frac{3}{2}}\,\ln\left|\frac{1+q''}{1-q''}\right|\right.$$

$$\left.+\,\frac{1}{q^2}\int_{1/q}^\infty dq''\,\frac{1}{q''^{\frac{1}{2}}}\,\ln\left|\frac{1+q''}{1-q''}\right|\,\right]$$

$$=\;8\pi^3 q^2\,\frac{1}{\sqrt{q^2+1}}\,\frac{1}{(\sqrt{q^2+1}+1)^2}\left[\pi\;-\;\frac{4}{5q^{\frac{1}{2}}}\ln\left|\frac{1+q}{1-q}\right|\right.$$

$$\left.+\left(\frac{2q^2}{5}-2\right)\arctan\frac{1}{\sqrt{q}}\;+\;\left(1\,-\,\frac{q^2}{5}\right)\ln\left|\frac{1+\sqrt{q}}{1-\sqrt{q}}\right|\;+\;\frac{4}{15}\sqrt{q}\,\right]. \tag{H.4}$$

Due to the above choice of $f(p)$, the r.h.s. of (H.4)$\sim q^{\frac{5}{2}}$ for $q\to 0$, assuring that its contribution to $M_2(q)$ defined below (I.5.28) is finite. The integrals occurring here and in the remaining contributions to T_2 are listed in Appendix A, starting from (A.11).

It should be noted that the Sobolev representation for the Jansen-Hess operator cannot be used in the virial theorem. The reason is that the transformation operators U_0' in (I.4.1) linking b_m and $B_m^{(2)}$ do depend on the mass m and hence influence the derivatives.

Appendix J

On the expectation value of F_0 in the positive spectral subspace

We will show that for the first-order expansion term F_0 of the exact projector P_+, one has $(\psi, F_0\,\psi) = 0$ if $\psi\in\mathcal{H}_{+,N}$.

For a state ψ in the positive spectral subspace of the free Dirac operator, one has for any $l\in\{1,...,N\}$: $\Lambda_+^{(l)}\,\psi = \psi$. Therefore the expectation value of $F_0^{(l)}$, l specifying the particle on which F_0 is acting, can be written in the form

$$(\psi, F_0^{(l)}\,\psi)\;=\;(\Lambda_+^{(l)}\,\psi, F_0^{(l)}\,\Lambda_+^{(l)}\,\psi)\;=\;(\psi,\Lambda_+^{(l)}\,F_0^{(l)}\,\Lambda_+^{(l)}\,\psi). \tag{J.1}$$

Dropping the index l again, we use the relation (I.3.26) between the symbol and the kernel of an operator to extract from (II.3.19)

$$k_{F_0}(\mathbf{p},\mathbf{p}')\;=\;-\frac{\gamma}{(2\pi)^2}\,\frac{1}{|\mathbf{p}-\mathbf{p}'|^2}\,\frac{1}{E_p+E_{p'}}\,(1\,-\,\tilde{D}_0(\mathbf{p})\,\tilde{D}_0(\mathbf{p}')) \tag{J.2}$$

such that the r.h.s. of (J.1) is written as

$$(\psi,\Lambda_+\,F_0\,\Lambda_+\,\psi)\;=\;-\frac{\gamma}{(2\pi)^2}\,\frac{1}{4}\int_{\mathbb{R}^{3N-3}}dQ\int d\mathbf{p}\,d\mathbf{p}'\,\frac{1}{|\mathbf{p}-\mathbf{p}'|^2}\,\frac{1}{E_p+E_{p'}}$$

$$\cdot \overline{\hat{\psi}_Q(\mathbf{p})}\,(1 + \tilde{D}_0(\mathbf{p}))\,(1 - \tilde{D}_0(\mathbf{p})\,\tilde{D}_0(\mathbf{p}'))\,(1 + \tilde{D}_0(\mathbf{p}'))\,\hat{\psi}_Q(\mathbf{p}'), \tag{J.3}$$

where Q comprises the coordinates (respective momenta) of the remaining $N-1$ particles. However, it is easily verified that

$$(1 + \tilde{D}_0(\mathbf{p}))\,(1 - \tilde{D}_0(\mathbf{p})\,\tilde{D}_0(\mathbf{p}'))\,(1 + \tilde{D}_0(\mathbf{p}')) \;=\; 0 \tag{J.4}$$

since $\tilde{D}_0^2 = 1$. Thus $(\psi, F_0\,\psi) \;= 0$.

We want to add that also $\Lambda_-\,F_0\,\Lambda_- = 0$, such that $F_0 \;= \Lambda_+\,F_0\,\Lambda_- + \Lambda_-\,F_0\,\Lambda_+$ is an odd operator. (However, $\|F_0\psi\| \neq 0$ for $\psi \in \mathcal{H}_{+,N}$, see section II.5.)

Define now a multi-particle operator $A^{(nk)}\,F_0^{(l)}$ with $l \neq n, k$. (In our case of interest, $A^{(nk)} := V^{(nk)}$.) Since for $\psi \in \mathcal{H}_{+,N}$ one has $\Lambda_+^{(l)}\psi = \psi$, the expectation value turns into

$$(\psi, A^{(nk)}\,F_0^{(l)}\,\psi) \;=\; (\psi, A^{(nk)}\,\Lambda_+^{(l)}\,F_0^{(l)}\,\Lambda_+^{(l)}\,\psi) \tag{J.5}$$

because $\Lambda_+^{(l)}$ commutes with $A^{(nk)}$ for distinct particles. However, the r.h.s. of (J.5) vanishes since $\Lambda_+^{(l)}\,F_0^{(l)}\,\Lambda_+^{(l)} \;= 0$ as shown above.

References

Abramowitz M. and Stegun I.A. 1965: *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables.* Dover Publications, New York

(BBHS) Bach V., Barbaroux J.M., Helffer B. and Siedentop H. 1999: On the stability of the relativistic electron-positron field. Commun. Math. Phys. **201**, 445-460

Balinsky A.A. and Evans W.D. 1998: On the virial theorem for the relativistic operator of Brown and Ravenhall, and the absence of embedded eigenvalues. Lett. Math. Phys. **44**, 233-248

Balinsky A.A. and Evans W.D. 1999: Stability of one-electron molecules in the Brown-Ravenhall model. Commun. Math. Phys. **202**, 481-500

Bethe H.A. and Salpeter E.E. 1957: *Quantum Mechanics of One and Two Electron Atoms.* Springer-Verlag, Berlin

Brown G.E. and Ravenhall D.G. 1951: On the interaction of two electrons. Proc. Roy. Soc. London **A208**, 552-559

(BSS) Brummelhuis R., Siedentop H. and Stockmeyer E. 2002: The ground state energy of relativistic one-electron atoms according to Jansen and Hess. Doc. Math. **7**, 167-182

Burenkov V.I. and Evans W.D. 1998: On the evaluation of the norm of an integral operator associated with the stability of one-electron atoms. Proc. Roy. Soc. (Edinburgh) **128A**, 993-1005

Darwin C.G. 1928: The wave equations of the electron. Proc. Roy. Soc. (London) **A118**, 654-679

Datta N., Fernández R. and Fröhlich J. 1999: Effective hamiltonians and phase diagrams for tight-binding models. Journal of Stat. Phys. **96**, 545-611

Dirac P.A.M. 1928: The quantum theory of the electron. Proc. Roy. Soc. London **A117**, 610-624

(DES) Dolbeault J., Esteban M.J. and Séré E. 2000: Variational characterisation for eigenvalues of Dirac operators. Calc. Var. **10**, 321-347

Douglas M. and Kroll N.M. 1974: Quantum electrodynamical corrections to the fine structure of helium. Ann. Phys. (N.Y.) **82**, 89-155

Durand Ph. and Malrieu J.-P. 1987: Effective Hamiltonians and pseudo potentials as tools for rigorous modelling. In *Ab initio Methods in Quantum Chemistry*, ed. I.K.P. Lawley, John Wiley and Sons, New York

(EPS) Evans W.D., Perry P. and Siedentop H. 1996: The spectrum of relativistic one-electron atoms according to Bethe and Salpeter. Commun. Math. Phys. **178**, 733-746

Foldy L.L. and Wouthuysen S.A. 1950: On the Dirac theory of spin $\frac{1}{2}$ particles and its non-relativistic limit. Phys. Rev. **78**, 29-36

Folland G.B. 1995: *Introduction to Partial Differential Equations*, 2^{nd} edition. Princeton University Press, Princeton

Gradshteyn I.S. and Ryzhik I.M. 1965: *Table of Integrals, Series and Products.* Academic Press, New York

Halmos P.R. and Sunder V.S. 1978: *Bounded Integral Operators on L^2 Spaces.* Springer-Verlag, Berlin

Herbst I.W. 1977: Spectral theory of the operator $(p^2 + m^2)^{\frac{1}{2}} - Ze^2/r$. Commun. Math. Phys. **53**, 285-294

Hess B.A. 1986: Relativistic electronic-structure calculations employing a two-component no-pair formalism with external-field projection operators. Phys. Rev. **A33**, 3742-3748

Hoever G. and Siedentop H. 1999: Stability of the Brown-Ravenhall operator. Math. Phys. Electron. J. **5**(6), 1-11

Hunziker W. 1966: On the spectra of Schrödinger multiparticle Hamiltonians. Helv. Phys. Acta **39**, 451-462

(IJA) Iantchenko A. and Jakubassa-Amundsen D.H. 2003: On the positivity of the Jansen-Hess operator for arbitrary mass. Ann. Henri Poincaré **4**, 1-17

(JA) Jakubassa-Amundsen D.H. 2002: The essential spectrum of relativistic one-electron ions in the Jansen-Hess model. Math. Phys. Electron. J. **8**(3), 1-30

Jansen G. and Hess B.A. 1989: Revision of the Douglas-Kroll transformation. Phys. Rev. **A39**, 6016-6017

Kadison R.V. and Ringrose J.R. 1983: *Fundamentals of the Theory of Operator Algebras* Vol. **1**. Academic Press, New York

Kato T. 1966: *Perturbation Theory for Linear Operators*, Vol. **132** of *Grundlehren der mathematischen Wissenschaften*. Springer-Verlag, Berlin

Landau L.D. and Lifschitz E.M. 1965: *Quantenmechanik*, Vol. **III** of *Lehrbuch der Theoretischen Physik*. Akademie-Verlag, Berlin

Lieb E.H. and Yau H.-T. 1988: The stability and instability of relativistic matter. Commun. Math. Phys. **118**, 177-213

Mittleman M.H. 1981: Theory of relativistic effects on atoms: Configuration-space Hamiltonian. Phys. Rev. **A24**, 1167-1175

Morse P.M. and Feshbach H. 1953: *Methods of Theoretical Physics* part **II**, §9. Mc Graw Hill, New York

Pauli W. 1927: Zur Quantenmechanik des magnetischen Elektrons. Z. Phys. **43**, 601-623

Pauli W. 1958: Die allgemeinen Prinzipien der Wellenmechanik, in *Handbuch der Physik*, Vol. **V** Teil 1. Springer-Verlag, Berlin, 1-168

Pearson D.B. 1988: *Quantum Scattering and Spectral Theory.* Academic Press, New York

Reed M. and Simon B. 1980: *Functional Analysis* Vol. **I** of *Methods of Modern Mathematical Physics.* Academic Press, New York

Reed M. and Simon B. 1978: *Analysis of Operators* Vol. **IV** of *Methods of Modern Mathematical Physics.* Academic Press, New York

Rose, E.M. 1961: *Relativistic Electron Theory.* John Wiley and Sons, New York

Sobolev A. 2003: Integrated density of states for the periodic Schrödinger operator in dimension two. University of Sussex preprint

Sobolev A. 2004: Asymptotics of the integrated density of states for periodic elliptic pseudo-differential operators in dimension one. Revista Matematica Iberoamericana, in print

Sucher J. 1958: PhD Thesis (Columbia University, USA)

Sucher J. 1987: Relativistic many-electron Hamiltonians. Phys. Scripta **36**, 271-281

Sucher J. 1980: Foundations of the relativistic theory of many-electron atoms. Phys. Rev. **A22**, 348-362

Stockmeyer E. 2002: Electrones relativistas en un contexto de la estabilidad de la materia. PhD Thesis (Pontificia Catholic Universiy of Chile)

Taylor M.E. 1981: *Pseudodifferential Operators.* Princeton University Press, Princeton

Thaller B. 1992: *The Dirac Equation.* Springer-Verlag, Berlin

Tix C. 1997: Self-adjointness and spectral properties of a pseudo-relativistic Hamiltonian due to Brown and Ravenhall. Preprint mp-arc/97-441

Tix C. 1998: Strict positivity of a relativistic Hamiltonian due to Brown and Ravenhall. Bull. London Math. Soc. **30**, 283-290

De Vries E. 1970: Foldy-Wouthuysen transformations and related problems. Fortschr. Physik **18**, 149-182

Weidmann J. 1980: *Linear Operators in Hilbert Spaces.* Springer-Verlag, Berlin

Werner D. 1995: *Funktionalanalysis.* Springer-Verlag, Berlin

Wolf A., Reiher M. and Hess B.A. 2002: The generalised Douglas-Kroll transformation. J. Chem. Phys. **117**, 9215-9226

Wolf A., Reiher M. and Hess B.A. 2004: Transgressing theory boundaries: The generalised Douglas-Kroll transformation. In *Recent Advances in Relativistic Effects in Chemistry*, eds. K. Hirao and Y. Ishikawa. World Scientific Publishing, Singapore. In print.

Notations

$\mathcal{A}$	antisymmetrisation with respect to interchange of two particles
$A^{(n)}$	operator A relating to the n-th particle
A^*	adjoint of operator A
$a(\mathbf{x},\mathbf{p})$	symbol of operator A, defined by $(A\varphi)(\mathbf{x}) = (2\pi)^{-\frac{3}{2}} \int d\mathbf{p}\, a(\mathbf{x},\mathbf{p})\, e^{i\mathbf{px}}\hat{\varphi}(\mathbf{p})$
$\hat{a}(\mathbf{q},\mathbf{p})$	Fourier transform of symbol with respect to $\mathbf{x}$
$[A,B]$	$AB - BA$ (commutator of A and B)
$\boldsymbol{\alpha}$	vector of Dirac matrices in $\mathbb{C}^{4,4}$
β	$\begin{pmatrix} I & \\ & -I \end{pmatrix} \in \mathbb{C}^{4,4}$
$\mathbb{C}$	complex space
D_0	free one-particle Dirac operator
$\tilde{D}_0$	$D_0/\|D_0\|$ (an operator of norm unity)
d_θ	dilation operator, defined by $d_\theta \hat{u}(\mathbf{p}) = \theta^{-\frac{3}{2}}\,\hat{u}(\mathbf{p}/\theta)$
$d\omega$	area element on the unit sphere S^2
$f^\#$	Mellin transform, defined by $f^\#(t) = (2\pi)^{-\frac{1}{2}} \int_0^\infty dp\, f(p)\, p^{-it-\frac{1}{2}}$
γ	potential strength
γ_{BR}	$2/(\frac{\pi}{2} + \frac{2}{\pi})$
γ_c	critical potential strength
γ_J	1.006
Γ	gamma function
H	$D_0 + V$ (Dirac operator)
$\mathcal{H}$	Hilbert space (complete metric space with scalar product)
$\mathcal{H}_{+,1}$	$\Lambda_+\,(H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4)$
$\mathcal{H}_{+,N}$	$\Lambda_+^{(1)} \otimes \cdots \otimes \Lambda_+^{(N)}\, \mathcal{A}(H_{1/2}(\mathbb{R}^3) \times \mathbb{C}^4)^N$, N the number of particles
$H_{1/2}(\mathbb{R}^3)$	Sobolev space of order 1/2 (form domain of D_0)
$H_1(\mathbb{R}^3)$	Sobolev space of order 1 (domain of D_0)
Im z	imaginary part of z
$k_A(\mathbf{p},\mathbf{p}')$	kernel of operator A, defined by $(A\varphi)(\mathbf{p}) = \int d\mathbf{p}'\, k_A(\mathbf{p},\mathbf{p}')\,\varphi(\mathbf{p}')$
$L_2(\mathbb{R}^3)$	Hilbert space of (equivalence class of) square-integrable functions with domain $\mathbb{R}^3$
Λ_+	projection onto the positive spectral subspace of D_0
Λ_-	projection onto the negative spectral subspace of D_0
$\mathbb{N}_0$	space of natural numbers $\mathbb{N} \cup \{0\}$
Ω_ν	vector spherical harmonic
ΨDO	pseudodifferential operator (defined by its symbol)
$\mathbb{R}$	real space
$\mathbb{R}_+$	positive real space
Re z	real part of z
$\mathcal{S}$	Schwartz space of infinitely differentiable, rapidly decreasing functions
$\sigma_1, \sigma_2, \sigma_3$	Pauli matrices in $\mathbb{C}^{2,2}$
$\sigma(H)$	spectrum of H
$\sigma_{ac}(H)$	absolutely continuous spectrum of H
$\sigma_{ess}(H)$	essential spectrum of H
$\sigma_p(H)$	point spectrum of H (set of eigenvalues of H)
$\sigma_{sc}(H)$	singular continuous spectrum of H
T	kinetic energy operator
T_a	translation operator, defined by $T_a\varphi(\mathbf{x}) = \varphi(\mathbf{x} + \mathbf{a})$

U_k	unitary transformation operator
V	$-\gamma/x$ (Coulomb potential), except in section I.2.d
Y_{lM}	spherical harmonic
$\mathbb{Z}_-$	space of negative integers
$(\,\cdot\,,\,\cdot\,)$	scalar product in the Hilbert space L_2
(φ, ϕ)	$\int d\mathbf{x}\,\overline{\varphi(\mathbf{x})}\,\phi(\mathbf{x})$
$\hat{\varphi}$	Fourier transform of φ
$(\hat{\varphi}, \hat{\phi})$	$\int d\mathbf{p}\,\overline{\hat{\varphi}(\mathbf{p})}\,\hat{\phi}(\mathbf{p}) \;=\; (\varphi, \phi)$
$\\|\ \\|$	norm in $L_2(\mathbb{R}^3)$
$\\|A\varphi\\|$	$(A\varphi, A\varphi)^{1/2}$
$\\|A\\|$	$\sup_{\\|\varphi\\|=1} \\|A\varphi\\|$

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