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CONSTRUCTION OF THE PAULI-VILLARS-REGULATED DIRAC VACUUM IN ELECTROMAGNETIC FIELDS

PHILIPPE GRAVEJAT, CHRISTIAN HAINZL, MATHIEU LEWIN, AND ÉRIC SÉRÉ

Abstract. Using the Pauli-Villars regularization and arguments from convex analysis, we construct the polarized Dirac vacuum, in the presence of small external electromagnetic fields. We describe the electrons by a Hartree-Fock-type theory and the photons by a self-consistent classical magnetic potential. The resulting vacuum polarization coincides on first order with that of full Quantum Electrodynamics.

Contents

1. Introduction

Quantum Electrodynamics (QED) is a powerful theory which describes the interactions of matter with light. Even if it is very well documented in the Physics literature, its mathematical properties are far from being fully understood. A non-perturbative rigorous formulation of QED is indeed still missing.

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One possibility to attack this fundamental problem is via Lattice QED [28, 35, 26]. With J.-P. Solovej, we followed another route in a series of works [17, 18, 20, 19, 14, 15] which originated from a fundamental paper of Chaix and Iracane [4]. We considered the simpler Hartree-Fock approximation of QED, in which only the instantaneous Coulomb interactions between particles are taken into account. We were able to study this model in the non-perturbative regime, that is for all values of the bare coupling constant $0 < \alpha < 4/\pi$. It is remarkable that this 'no-photon' mean-field theory can be formulated in a fully non-perturbative way, but certainly disappointing that transversal quantized photons have been neglected. The purpose of the present work is to make a first step towards the inclusion of photons in Hartree-Fock QED, by considering the interaction of Dirac's vacuum with classical, but optimized, electromagnetic fields. This is equivalent to assuming that photons are described by a coherent state in Fock space (the simpler mean-field approximation for bosons). Our theory will be based on a famous regularization procedure introduced by Pauli and Villars in [29].

1.1. **Hamiltonian and Lagrangian formalism.** We explain here the origin of the model. Our starting point is the *formal* Hamiltonian of QED, written in Coulomb gauge, in the presence of an external electromagnetic four-potential $\boldsymbol{A}_{\rm ext} := (V_{\rm ext}, A_{\rm ext})$, see [22, 23, 38, 33, 3, 19],

$$\begin{aligned}\mathbb{H}^{\boldsymbol{A}_{\rm ext}} = \int \Psi^*(x)\Big[\boldsymbol{\alpha}\cdot(-i\nabla - e\mathbb{A}(x) - eA_{\rm ext}(x)) + m\boldsymbol{\beta}\Big]\Psi(x)\,dx \\ + e\int V_{\rm ext}(x)\rho(x)\,dx + \frac{e^2}{2}\iint \frac{\rho(x)\rho(y)}{|x-y|}dx\,dy + \mathbb{H}_f.\end{aligned} \tag{1.1}$$

Here the four Dirac matrices $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \boldsymbol{\alpha}_3)$ and $\boldsymbol{\beta}$ are equal to

$$\boldsymbol{\alpha}_k := \begin{pmatrix} 0 & \boldsymbol{\sigma}_k \\ \boldsymbol{\sigma}_k & 0 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\beta} := \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix},$$

the Pauli matrices $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$ and $\boldsymbol{\sigma}_3$ being defined by

$$\boldsymbol{\sigma}_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\sigma}_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For later purposes we introduce the Dirac operator with mass m and electromagnetic four-potential $\boldsymbol{A} = (V, A)$,

$$D_{m,e\boldsymbol{A}} := \boldsymbol{\alpha}\cdot\big(-i\nabla - eA(x)\big) + eV(x) + m\boldsymbol{\beta}. \tag{1.2}$$

In Formula (1.1), $\Psi(x)$ is the second quantized field operator which annihilates an electron at x and satisfies the anti-commutation relation

$$\Psi^*(x)_\sigma\Psi(y)_\nu + \Psi(y)_\nu\Psi^*(x)_\sigma = 2\delta_{\sigma,\nu}\delta(x-y). \tag{1.3}$$

Here $\Psi(x)_\sigma$ is an operator-valued distribution. The operator $\rho(x)$ is the *density operator* defined by

$$\rho(x) := \frac{1}{2}\sum_{\sigma=1}^{4}[\Psi^*_\sigma(x), \Psi_\sigma(x)], \tag{1.4}$$

where $[a,b] := ab - ba$. The operator $\mathbb{H}_f$ in (1.1) describes the kinetic energy of the photons given by

$$\mathbb{H}_f = \frac{1}{8\pi}\int |\operatorname{curl} \mathbb{A}(x)|^2\,dx = \sum_{\lambda=1,2}\int_{\mathbb{R}^3} |k| a^*_\lambda(k) a_\lambda(k)\,dk + \text{Cst},$$

where Cst indicates a constant which diverges in infinite volume. The vector $\mathbb{A}(x)$ is the magnetic field operator for the photons and $a^*_\lambda(k)$ is the creation operator of a photon with momentum k and polarization λ. The Hamiltonian $\mathbb{H}^{\boldsymbol{A}_{\rm ext}}$ formally acts on the Fock space $\mathcal{F} = \mathcal{F}_{\rm e} \otimes \mathcal{F}_{\rm ph}$ where $\mathcal{F}_{\rm e}$ is the fermionic Fock space for the electrons and $\mathcal{F}_{\rm ph}$ is the bosonic Fock space for the photons.

We now restrict the above (formal) Hamiltonian to states of the special form

$$\Omega = \Omega_{\rm HF} \otimes \Omega_{\rm Coh},$$

where $\Omega_{\rm HF}$ is an electronic (generalized) Hartree-Fock state characterized by its one-particle density matrix $0 \leq \gamma \leq 1$, and $\Omega_{\rm Coh}$ is a coherent state characterized by its magnetic potential $A(x)$ (a given classical vector field on $\mathbb{R}^3$). In other terms, $\gamma(x,y) = \langle \Psi^*(x)\Psi(y)\rangle_{\Omega_{\rm HF}}$, and $A(x) = \langle \mathbb{A}(x)\rangle_{\Omega_{\rm Coh}}$. The coherent state $\Omega_{\rm Coh}$ is always pure but the generalized Hartree-Fock state $\Omega_{\rm HF}$ is mixed when γ is not an orthogonal projection [2]. Computing the corresponding energy yields (up to a universal constant which diverges in infinite volume)

$$\begin{aligned}\langle \mathbb{H}^{\boldsymbol{A}_{\rm ext}}\rangle_\Omega = {}& \operatorname{tr}\Big\{\Big(\boldsymbol{\alpha}\cdot(-i\nabla - eA - eA_{\rm ext}) + m\boldsymbol{\beta}\Big)(\gamma - 1/2)\Big\}\\ &+ e\int_{\mathbb{R}^3} V_{\rm ext}(x)\rho_{\gamma-1/2}(x)\,dx + \frac{e^2}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\rho_{\gamma-1/2}(x)\rho_{\gamma-1/2}(y)}{|x-y|}\,dx\,dy\\ &- \frac{e^2}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|(\gamma-1/2)(x,y)|^2}{|x-y|}\,dx\,dy + \frac{1}{8\pi}\int_{\mathbb{R}^3}|\operatorname{curl} A(x)|^2\,dx,\end{aligned}$$

see [20] for some computational details. The nonlinear terms appearing on the second and third lines are the so-called *direct* and *exchange* terms. That the energy depends on $\gamma - 1/2$ is due to the charge-conjugation invariant choice (1.4) for the density operator $\rho(x)$.

It is more convenient to express the previous energy by introducing the Coulomb potential V induced by the density $\rho_{\gamma-1/2}$ and which solves Poisson's equation

$$-\Delta V = 4\pi e\,\rho_{\gamma-1/2}, \tag{1.5}$$

that is,

$$V(x) = e\int_{\mathbb{R}^3}\frac{\rho_{\gamma-1/2}(y)}{|x-y|}\,dy.$$

We can then write

$$\begin{aligned}&\frac{e^2}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\rho_{\gamma-1/2}(x)\rho_{\gamma-1/2}(y)}{|x-y|}\,dx\,dy\\ &\qquad = e\int_{\mathbb{R}^3}\rho_{\gamma-1/2}(x)\,V(x)\,dx - \frac{1}{8\pi}\int_{\mathbb{R}^3}|\nabla V(x)|^2\,dx.\end{aligned}$$

Indeed, the potential V solving (1.5) is the unique solution to the maximization problem

$$\frac{e^2}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\rho_{\gamma-1/2}(x)\rho_{\gamma-1/2}(y)}{|x-y|}\,dx\,dy \\ = \sup_V\left\{e\int_{\mathbb{R}^3}\rho_{\gamma-1/2}(x)\,V(x)\,dx - \frac{1}{8\pi}\int_{\mathbb{R}^3}|\nabla V(x)|^2\,dx\right\}.$$

It is a useful technique to introduce an auxiliary unknown field V which can vary freely, and over which the functional is maximized in the end. Introducing the (time-independent) four potential $\boldsymbol{A} := (V, A)$, we arrive at the Hartree-Fock Lagrangian

$$\operatorname{tr}\left(D_{m,e(\boldsymbol{A}+\boldsymbol{A}_{\rm ext})}(\gamma-1/2)\right) - \frac{e^2}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|(\gamma-1/2)(x,y)|^2}{|x-y|}\,dx\,dy \\ + \frac{1}{8\pi}\int_{\mathbb{R}^3}\left(|\operatorname{curl}A(x)|^2 - |\nabla V(x)|^2\right)dx.$$

All the terms in this expression are actually infinite, but they make sense when the system is restricted to a box with an ultraviolet cut-off.

We now neglect the exchange term, that is we work in reduced Hartree-Fock (rHF) theory. This leads us to considering the rHF Lagrangian

$$\mathcal{L}_{\rm rHF}^{\boldsymbol{A}_{\rm ext}}(\gamma,\boldsymbol{A}) = \operatorname{tr}\left(D_{m,e(\boldsymbol{A}+\boldsymbol{A}_{\rm ext})}(\gamma-1/2)\right) \\ + \frac{1}{8\pi}\int_{\mathbb{R}^3}\left(|\operatorname{curl}A(x)|^2 - |\nabla V(x)|^2\right)dx. \tag{1.6}$$

It will be clearer later why the no-exchange model is easier to handle. In relativistic density functional theory [10], this term would be approximated by a function of $\rho_{\gamma-1/2}$ only.

Remark 1.1. Another way to derive the same rHF Lagrangian (1.6) is to start from the formal Lagrangian of QED [33], with a *classical* electromagnetic field instead of a quantized one. In the time-independent case one arrives at (1.6) (with a different sign). Since there are only one-body potentials in this model, the electrons are automatically in a Hartree-Fock state and no further approximation is necessary. This approach was undertaken by J. Schwinger in his celebrated paper [34] on vacuum polarization, where he derived the probability of pair creation by tunneling in a strong electrostatic field. The functional defined in this paper is therefore suitable for a rigorous examination of this so-called *Schwinger effect*.

1.2. **The self-consistent equations.** Our goal is to construct rHF ground states. They are obtained by minimizing the functional (1.6) with respect to both the electronic density matrix γ and the classical photon field A, and maximizing over V. If no constraint (other than the Pauli principle $0 \le \gamma \le 1$) is imposed on γ, then we are considering the rHF polarized vacuum in the presence of the external field $\boldsymbol{A}_{\rm ext}$. For atoms and molecules, a charge constraint of the form

$$\operatorname{tr}\left(\gamma - \frac{1}{2}\right) = N,$$

is needed. In this paper we restrict ourselves to the vacuum case.

Any optimal state is a formal solution of the following self-consistent equations

$$\begin{cases} \gamma = \mathbb{1}_{(-\infty,0)}\Big(\boldsymbol{\alpha}\cdot(-i\nabla - eA - eA_{\rm ext}) + m\boldsymbol{\beta} + eV + eV_{\rm ext}\Big), \\ -\Delta A = 4\pi\, e\, j_{\gamma-1/2}, \\ -\Delta V = 4\pi\, e\, \rho_{\gamma-1/2}, \\ \operatorname{div} A = \operatorname{div} A_{\rm ext} = 0, \end{cases} \tag{1.7}$$

where

$$j_{\gamma-1/2}(x) = \operatorname{tr}_{\mathbb{C}^4}\Big(\boldsymbol{\alpha}\Big(\gamma - \frac{1}{2}\Big)(x,x)\Big),$$

and

$$\rho_{\gamma-1/2}(x) = \operatorname{tr}_{\mathbb{C}^4}\Big(\Big(\gamma - \frac{1}{2}\Big)(x,x)\Big),$$

are respectively the current and charge density of the polarized vacuum. The equation on γ (the first line of (1.7)) means that the polarized vacuum consists of particles filling all the negative energies of the mean-field Dirac operator (appearing in the parenthesis), in accordance with the original ideas of Dirac [6, 7, 8]. The equations (1.7) are well-known in the literature, see, e.g., [10, Eq. (62)-(64)]. For atoms and molecules, the vacuum projection $\mathbb{1}_{(-\infty,0)}(\cdots)$ has to be replaced by a spectral projection of the form $\mathbb{1}_{(-\infty,\mu)}(\cdots)$, for some chemical potential μ which is chosen to ensure the correct number N of electrons in the gap (more precisely the correct total charge of the system). Except from this change of chemical potential, the equations take exactly the same form.

1.3. **The Pauli-Villars regularization.** After having discussed the general idea of the method, we now present the technique that we have employed to give it a rigorous meaning. First, it is not obvious whether we are solving the same problem when we change the order of the minimization in A and γ and the maximization in V. Since the theory is divergent for large momenta, we will have to put some ultraviolet cut-off. This regularization might also not commute with the $\min_\gamma$, $\min_A$ and $\max_V$. In this paper we choose the following route:

(1) We minimize with respect to the density matrix γ and obtain a formal Lagrangian action functional depending on V and A only;
(2) We regularize the functional by using the Pauli-Villars scheme [29];
(3) We finally show that the order of the $\min_A$ and $\max_V$ do not matter, and we prove the existence of a corresponding (unique) saddle point. This unique state is the free vacuum when $\boldsymbol{A}_{\rm ext} \equiv 0$ and it is the polarized vacuum when $\boldsymbol{A}_{\rm ext} \neq 0$.

Summarizing, we solve the following variational problem:

$$\max_V \min_A \underbrace{\Big(\min_\gamma \mathcal{L}^{\boldsymbol{A}_{\rm ext}}_{\rm rHF}(\gamma,V,A)\Big)}_{\rm Pauli-Villars-regulated} = \min_A \max_V \underbrace{\Big(\min_\gamma \mathcal{L}^{\boldsymbol{A}_{\rm ext}}_{\rm rHF}(\gamma,V,A)\Big)}_{\rm Pauli-Villars-regulated},$$

for $\boldsymbol{A}_{\rm ext} \equiv 0$ and for $\boldsymbol{A}_{\rm ext} \neq 0$. The main advantage of our approach is that the minimization with respect to γ can be solved explicitly, since the functional is linear in γ. In principle the same technique could be used to

handle the exchange term (or a density functional approximation of it) as well. However, the minimization over γ becomes nonlinear in this case.

When $\boldsymbol{A} = \boldsymbol{A}_{\rm ext} = 0$, the formal solution of

$$\min_\gamma \mathcal{L}^0_{\rm rHF}(\gamma, 0, 0) = \min_\gamma \operatorname{tr}\Big(D_{m,0}\Big(\gamma - \frac{1}{2}\Big)\Big),$$

is the free Dirac sea

$$\gamma = P^0_- = \mathbb{1}_{(-\infty,0)}\big(D_{m,0}\big).$$

The electrons fill in completely the negative Dirac energies. The corresponding energy, namely

$$\begin{aligned}\operatorname{tr}\Big(D_{m,0}\Big(\gamma - \frac{1}{2}\Big)\Big) &= \frac{1}{2}\operatorname{tr} D_{m,0}\left(\mathbb{1}_{(-\infty,0)}\big(D_{m,0}\big) - \mathbb{1}_{(0,\infty)}\big(D_{m,0}\big)\right)\\ &= -\frac{1}{2}\operatorname{tr}\big|D_{m,0}\big|,\end{aligned}$$

is infinite, except if we are in a box with an ultraviolet cut-off.

Here and everywhere in the paper, the absolute value of an operator is defined by the functional calculus

$$|A| := \sqrt{A^* A}.$$

It is in general not a scalar operator, that is, it may still depend on the spin. In the special case of $D_{m,0}$, it does not depend on the spin, however, since it is the scalar pseudo-differential operator

$$\big|D_{m,0}\big| = \sqrt{-\Delta + m^2}.$$

In the general case, the formal solution is

$$\gamma = \mathbb{1}_{(-\infty,0)}\big(D_{m,e(\boldsymbol{A}+\boldsymbol{A}_{\rm ext})}\big),$$

and the associated minimum is

$$\min_\gamma \mathcal{L}^{\boldsymbol{A}_{\rm ext}}_{\rm rHF}(\gamma, V, A) = -\frac{1}{2}\operatorname{tr}\big|D_{m,e(\boldsymbol{A}+\boldsymbol{A}_{\rm ext})}\big| + \frac{1}{8\pi}\int_{\mathbb{R}^3}\big(|\operatorname{curl} A|^2 - |\nabla V|^2\big). \tag{1.8}$$

Again this quantity is always infinite. However, it can be given a clear mathematical meaning as follows. First, we can subtract the (infinite) energy of the free Dirac sea and define the relative Lagrangian as

$$\mathscr{L}^{\boldsymbol{A}_{\rm ext}}_{\rm rel}(\boldsymbol{A}) := \frac{1}{2}\operatorname{tr}\Big(\big|D_{m,0}\big| - \big|D_{m,e(\boldsymbol{A}+\boldsymbol{A}_{\rm ext})}\big|\Big) + \frac{1}{8\pi}\int_{\mathbb{R}^3}\big(|\operatorname{curl} A|^2 - |\nabla V|^2\big). \tag{1.9}$$

Since we have removed an (infinite) constant, we formally do not change the initial variational problem in which we are interested, hence we also do not change the self-consistent equations. Unfortunately, this functional is not yet well-defined, because the model is known to have important ultraviolet divergences. Indeed, the operator $|D_{m,0}| - |D_{m,e(\boldsymbol{A}+\boldsymbol{A}_{\rm ext})}|$ is not trace-class when $A+A_{\rm ext} \neq 0$ and its trace is not well-defined. This is reminiscent of the fact that the difference of the two corresponding negative projectors is never Hilbert-Schmidt [27]. In order to remove these divergences, an ultraviolet cut-off has to be imposed. The choice of this regularization is extremely important. Some simple choices in the spirit of what we have done in the purely electrostatic case (see, e.g. [14] for two different choices) would not work here, because of their lack of gauge symmetry.

In 1949, Pauli and Villars [29] have proposed a very clever way to regularize QED, while keeping the appropriate invariances. It is this technique that we will use in this paper (but there are other choices). In our language,[1] it consists in introducing the following Lagrangian functional

$$\begin{aligned}\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(\boldsymbol{A}) := \frac{1}{2}\,\mathrm{tr}\left(\sum_{j=0}^{J} c_j\left(\left|D_{m_j,0}\right| - \left|D_{m_j,e(\boldsymbol{A}+\boldsymbol{A}_{\rm ext})}\right|\right)\right)\\ + \frac{1}{8\pi}\int_{\mathbb{R}^3}\left(|\operatorname{curl} A|^2 - |\nabla V|^2\right).\end{aligned} \tag{1.10}$$

Here $m_0 = m$ and $c_0 = 1$, whereas the other c_j and m_j describe fictitious particles with very large masses $m_j \gg 1$ such that

$$\sum_{j=0}^{J} c_j = \sum_{j=0}^{J} c_j\, m_j^2 = 0. \tag{1.11}$$

The role of this constraint is to remove the worst ultraviolet divergences.[2] We will show in this paper that it does actually remove divergences since we can define the trace of $\sum_{j=0}^{J} c_j(|D_{m_j,0}| - |D_{m_j,e(\boldsymbol{A}+\boldsymbol{A}_{\rm ext})}|)$ under these conditions.

The purpose of this paper is twofold. First we prove that $\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(\boldsymbol{A})$ can be properly defined under the natural conditions that the fields $B = \operatorname{curl} A$, $B_{\rm ext} = \operatorname{curl} A_{\rm ext}$, $E = -\nabla V$ and $E_{\rm ext} = -\nabla V_{\rm ext}$ have a finite energy, i.e. are square integrable, and that

$$\operatorname{div} A_{\rm ext} = \operatorname{div} A = 0,$$

which is the Coulomb gauge condition. We then show that

$$\mathscr{L}_{\rm PV}^{0}(0,0) = \max_{V} \mathscr{L}_{\rm PV}^{0}(V,0) = \min_{A} \mathscr{L}_{\rm PV}^{0}(0,A), \tag{1.12}$$

for V (resp. A) varying in a neighborhood of 0 for the norm $\|\nabla V\|_{L^2(\mathbb{R}^3)}$ (resp. $\|\operatorname{curl} A\|_{L^2(\mathbb{R}^3)}$). The interpretation of (1.12) is that the free vacuum $\gamma = P_-^0$ is stationary under its own electromagnetic excitations. We conjecture that it is also a global saddle point, but we are unable to prove this with our present technology.

In a second step, we show that the functional $\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}$ admits a local saddle point in a neighborhood of 0, when the norms $\|E_{\rm ext}\|_{L^2(\mathbb{R}^3)}$ and $\|B_{\rm ext}\|_{L^2(\mathbb{R}^3)}$ are sufficiently small. This proves the existence of the polarized vacuum in weak external electromagnetic fields. This state is not a solution to the original equations (1.7), but instead it solves the *Pauli-Villars regulated*

[1] If we describe the fictitious particles by the density matrices γ_j, with $\gamma_0 = \gamma$, then the Pauli-Villars scheme consists in optimizing the functional $\sum_{j=0}^{J} c_j\ \mathrm{tr}\, D_{m_j,e(\boldsymbol{A}+\boldsymbol{A}_{\rm ext})}(\gamma_j - 1/2)$, subject to the Pauli principles $0 \le \gamma_j \le 1$. The energy must be minimized over the matrices γ_j such that $c_j > 0$ and maximized over those such that $c_j < 0$. Adding the infinite constant $\sum_{j=0}^{J} c_j\ \mathrm{tr}\,|D_{m_j,0}|/2$ gives Formula (1.10).

[2] More precisely, the role of (1.11) is to remove the *linear* ultraviolet divergence. The model is still logarithmically divergent, see (2.9) below.

equations

$$\begin{cases} Q = \sum\limits_{j=0}^{2} c_j \mathbb{1}_{(-\infty,0)}\Big(\boldsymbol{\alpha}\cdot(-i\nabla - eA - eA_{\rm ext}) + m_j\boldsymbol{\beta} + eV + eV_{\rm ext}\Big), \\ -\Delta A = 4\pi\, e\, j_Q, \\ -\Delta V = 4\pi\, e\, \rho_Q, \\ \operatorname{div} A = \operatorname{div} A_{\rm ext} = 0. \end{cases} \tag{1.13}$$

Our approach to prove the existence of such solutions consists in expanding the energy in powers of the elementary charge e. All the odd order terms vanish (by charge-conjugation invariance). Then we compute explicitly the second order term which is responsible of the ultraviolet divergences. It is important for our existence proof that this term be strictly convex in A and strictly concave in V. We also have to deal with the fourth order term in some detail. The latter was computed in the Physics literature in [24] and our task will be to estimate it. The higher order terms are then bounded in a rather crude way, following techniques of [17]. The main difficulty in our work is to verify that the Pauli-Villars conditions (1.11) induce the appropriate cancellations in the few first order terms, and to estimate them using the L^2–norm of the electromagnetic fields and nothing else.

In spite of its widespread use in quantum electrodynamics, the Pauli-Villars scheme [29] has not attracted a lot of attention on the mathematical side so far (see [12, 40, 41, 42, 11] for some previous results). The results of this paper seem to be among the first in this direction.

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2. Main results

Our goal is to study the Pauli-Villars Lagrangian functional which is formally given by

$$\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(\boldsymbol{A}) := \frac{1}{2}\operatorname{tr}\sum_{j=0}^{2} c_j\Big(\big|D_{m_j,0}\big| - \big|D_{m_j,e(\boldsymbol{A}+\boldsymbol{A}_{\rm ext})}\big|\Big) + \frac{1}{8\pi}\int_{\mathbb{R}^3}\big(|B|^2 - |E|^2\big), \tag{2.1}$$

where we recall that $B := \operatorname{curl} A$, $E := -\nabla V$, and

$$D_{m,e(\boldsymbol{A}+\boldsymbol{A}_{\rm ext})} := \boldsymbol{\alpha}\cdot\big(-i\nabla - e(A + A_{\rm ext})\big) + e(V + V_{\rm ext}) + m\boldsymbol{\beta}.$$

In Section 2.1, we recall some elementary spectral properties of $D_{m,\boldsymbol{A}}$ when the field $\boldsymbol{F} = (-\nabla V, \operatorname{curl} A)$ associated to $\boldsymbol{A} = (V, A)$ has a finite energy. In Section 2.2, we properly define the nonlinear term in (2.1), whereas in Sections 2.3 and 2.4, we show the existence of a saddle point for this functional, either when $\boldsymbol{A}_{\rm ext} \equiv 0$, or when $\boldsymbol{A}_{\rm ext} \neq 0$ is small enough.

2.1. **Elementary properties of electromagnetic Dirac operators.** Before entering the main subject of this article, we recall some elementary spectral properties of the Dirac operator in the presence of electromagnetic fields [43, Chap. 4]. The natural space in our setting is the Coulomb-gauge homogeneous Sobolev space

$$\dot{H}^1_{\rm div}(\mathbb{R}^3) := \Big\{ \boldsymbol{A} = (V, A) \in L^6(\mathbb{R}^3, \mathbb{R}^4) \ : \\ \operatorname{div} A = 0 \text{ and } \boldsymbol{F} = (-\nabla V, \operatorname{curl} A) \in L^2(\mathbb{R}^3, \mathbb{R}^6) \Big\}, \quad (2.2)$$

endowed with its norm

$$\|\boldsymbol{A}\|^2_{\dot{H}^1_{\rm div}(\mathbb{R}^3)} := \|\nabla V\|^2_{L^2(\mathbb{R}^3)} + \|\operatorname{curl} A\|^2_{L^2(\mathbb{R}^3)} = \|\boldsymbol{F}\|^2_{L^2(\mathbb{R}^3)}. \quad (2.3)$$

Here and everywhere, the equation $\operatorname{div} A = 0$ is understood in the sense of distributions.

Lemma 2.1 (Elementary spectral properties of $D_{m,\boldsymbol{A}}$)**.** *Let $m > 0$.*

(i) Any four-potential $\boldsymbol{A} \in \dot{H}^1_{\rm div}(\mathbb{R}^3)$ is $D_{m,0}$–compact. The operator $D_{m,\boldsymbol{A}}$ is self-adjoint on $H^1(\mathbb{R}^3)$ and its essential spectrum is

$$\sigma_{\rm ess}(D_{m,\boldsymbol{A}}) = (-\infty, -m] \cup [m, \infty).$$

(ii) The eigenvalues of $D_{m,\boldsymbol{A}}$ in $(-m, m)$ are Lipschitz functions of $\boldsymbol{A}$ in the norm $\|\boldsymbol{A}\|_{\dot{H}^1_{\rm div}(\mathbb{R}^3)}$.

(iii) There exists a universal constant C such that, if

$$\|\boldsymbol{A}\|_{\dot{H}^1_{\rm div}(\mathbb{R}^3)} \leq \eta\sqrt{m}, \quad (2.4)$$

for some number $\eta < 1/C$, then

$$\sigma(D_{m,\boldsymbol{A}}) \cap (-m(1 - C\eta), (1 - C\eta)m) = \emptyset.$$

(iv) Finally, if $V \equiv 0$, then $\sigma(D_{m,\boldsymbol{A}}) \cap (-m, m) = \emptyset$.

Proof. Recall the Kato-Seiler-Simon inequality [36, 39]

$$\forall p \geq 2, \ \big\|f(x)g(-i\nabla)\big\|_{\mathfrak{S}_p} \leq \frac{1}{(2\pi)^{\frac{3}{p}}} \big\|f\big\|_{L^p} \big\|g\big\|_{L^p}, \quad (2.5)$$

where $\mathfrak{S}_p$ is the usual Schatten class [39]. Applying (2.5) with $p = 6$ together with the Sobolev inequality, we obtain

$$\Big\| V \frac{1}{D_{m,0}} \Big\|_{\mathfrak{S}_6} \leq \frac{C}{\sqrt{m}} \big\|V\big\|_{L^6} \leq \frac{C}{\sqrt{m}} \big\|\nabla V\big\|_{L^2},$$

and, similarly,

$$\Big\| \boldsymbol{\alpha} \cdot A \frac{1}{D_{m,0}} \Big\|_{\mathfrak{S}_6} \leq \frac{C}{\sqrt{m}} \big\|A\big\|_{L^6} \leq \frac{C}{\sqrt{m}} \big\|\operatorname{curl} A\big\|_{L^2},$$

where we have used that $\operatorname{div} A = 0$. Since all the operators in $\mathfrak{S}_6$ are compact, statements *(i)* and *(ii)* follow from usual perturbation theory [25, 32]. Concerning *(iii)*, we notice that

$$D_{m,\boldsymbol{A}} \, (D_{m,0})^{-1} = \Big(I + \big(V - \boldsymbol{\alpha} \cdot A\big) \frac{1}{D_{m,0}} \Big)$$

so that, under condition (2.4),

$$\big|D_{m,\boldsymbol{A}}\big| \geq \big(1 - C\eta\big)\big|D_{m,0}\big|.$$

Statement (iii) then follows from (i), whereas (iv) is [43, Thm 7.1]. □

2.2. **Rigorous definition of the electron-positron energy.** Here, we explain how to provide a rigorous meaning to the functional

$$\boxed{\mathcal{F}_{\rm PV}\big(\boldsymbol{A}\big) := \frac{1}{2}\operatorname{tr}\sum_{j=0}^{2} c_j\Big(\big|D_{m_j,0}\big| - \big|D_{m_j,\boldsymbol{A}}\big|\Big)} \tag{2.6}$$

for a general four-potential $\boldsymbol{A} = (V, A)$ in the energy space $\dot{H}^1_{\rm div}(\mathbb{R}^3)$ (and which therefore satisfies the Coulomb gauge condition $\operatorname{div} A = 0$). Note that the first term in our functional (2.1) is nothing else but $\mathcal{F}_{\rm PV}(e(\boldsymbol{A} + \boldsymbol{A}_{\rm ext}))$.

As we have said, in Formula (2.6), the index $j = 0$ corresponds to the physical electron-positron field, while the other indices $j = 1, 2$ describe fictitious heavy particle fields. In particular, $m_0 > 0$ is the (bare) mass of the electron. We always take

$$c_0 = 1.$$

The role of the auxiliary particle fields is to provide an ultraviolet regularization. It is well-known in the Physics literature [29, 16, 3] that a sufficient condition to properly regularize the model is that the coefficients c_j and the masses m_j appearing in (2.1) satisfy

$$\boxed{\sum_j c_j = \sum_j c_j m_j^2 = 0.} \tag{2.7}$$

For this condition to be fulfilled, at least two additional distinct masses m_1 and m_2 are necessary. When there are exactly two fictitious fields, the condition (2.7) is equivalent to

$$c_1 = \frac{m_0^2 - m_2^2}{m_2^2 - m_1^2} \quad \text{and} \quad c_2 = \frac{m_1^2 - m_0^2}{m_2^2 - m_1^2}. \tag{2.8}$$

We will always assume that $m_0 < m_1 < m_2$, which implies that $c_1 < 0$ and $c_2 > 0$.

In the limit $m_1, m_2 \to \infty$, the regularization does not prevent a logarithmic divergence, which is best understood in terms of the averaged ultraviolet cut-off Λ defined as

$$\boxed{\log(\Lambda^2) := -\sum_{j=0}^{2} c_j \log(m_j^2).} \tag{2.9}$$

The value of Λ does not determine m_1 and m_2 uniquely. In practice, the latter are chosen as functions of Λ such that c_1 and c_2 remain bounded when Λ goes to infinity.

As we now explain, the Pauli-Villars regularization allows to give a rigorous meaning to the nonlinear term $\mathcal{F}_{\rm PV}$ defined in (2.6).

Theorem 2.1 (Proper definition of $\mathcal{F}_{\rm PV}$)**.** *Assume that c_j and m_j satisfy*

$$c_0 = 1, \quad m_2 > m_1 > m_0 > 0 \quad \text{and} \quad \sum_{j=0}^{2} c_j = \sum_{j=0}^{2} c_j m_j^2 = 0. \tag{2.10}$$

(i) Let

$$T_{\boldsymbol{A}} := \frac{1}{2} \sum_{j=0}^{2} c_j \Big(\big| D_{m_j,0} \big| - \big| D_{m_j,\boldsymbol{A}} \big| \Big). \tag{2.11}$$

For any $\boldsymbol{A} \in L^1(\mathbb{R}^3, \mathbb{R}^4) \cap \dot{H}^1_{\rm div}(\mathbb{R}^3)$, the operator $\mathrm{tr}_{\mathbb{C}^4} T_{\boldsymbol{A}}$ is trace-class on $L^2(\mathbb{R}^3, \mathbb{C})$. In particular, $\mathcal{F}_{\rm PV}(\boldsymbol{A})$ is well-defined in this case, by

$$\boxed{\mathcal{F}_{\rm PV}(\boldsymbol{A}) = \mathrm{tr}\, \big(\mathrm{tr}_{\mathbb{C}^4} T_{\boldsymbol{A}} \big).} \tag{2.12}$$

(ii) The functional $\mathcal{F}_{\rm PV}$ can be uniquely extended to a continuous mapping on $\dot{H}^1_{\rm div}(\mathbb{R}^3)$.

(iii) Let $\boldsymbol{A} \in \dot{H}^1_{\rm div}(\mathbb{R}^3)$. We have

$$\boxed{\mathcal{F}_{\rm PV}(\boldsymbol{A}) = \mathcal{F}_2(\boldsymbol{F}) + \mathcal{R}(\boldsymbol{A}),} \tag{2.13}$$

where $\boldsymbol{F} := (E, B)$, with $E = -\nabla V$ and $B = \mathrm{curl}\, A$. The functional $\mathcal{R}$ is continuous on $\dot{H}^1_{\rm div}(\mathbb{R}^3)$ and satisfies

$$|\mathcal{R}(\boldsymbol{A})| \leq K \left(\left(\sum_{j=0}^{2} \frac{|c_j|}{m_j} \right) \|\boldsymbol{F}\|_{L^2}^4 + \left(\sum_{j=0}^{2} \frac{|c_j|}{m_j^2} \right) \|\boldsymbol{F}\|_{L^2}^6 \right), \tag{2.14}$$

for a universal constant K.

(iv) The functional $\mathcal{F}_2$ is the non-negative and bounded quadratic form on $L^2(\mathbb{R}^3, \mathbb{R}^4)$ given by

$$\mathcal{F}_2(\boldsymbol{F}) = \frac{1}{8\pi} \int_{\mathbb{R}^3} M(k) \Big(\big| \widehat{B}(k) \big|^2 - \big| \widehat{E}(k) \big|^2 \Big)\, dk, \tag{2.15}$$

where

$$M(k) := -\frac{2}{\pi} \sum_{j=0}^{2} c_j \int_0^1 u(1-u) \log \big(m_j^2 + u(1-u)|k|^2 \big)\, du. \tag{2.16}$$

The function M is positive and satisfies the uniform estimate

$$0 < M(k) \leq M(0) = \frac{2 \log(\Lambda)}{3\pi}, \tag{2.17}$$

where Λ was defined previously in (2.9)*.*

Let us emphasize the presence of the $\mathbb{C}^4$–trace in statement (i) about the trace-class property of $\mathrm{tr}_{\mathbb{C}^4} T_{\boldsymbol{A}}$. We do not believe that the operator is trace-class without taking first the $\mathbb{C}^4$–trace, except when $V \equiv 0$. If we are allowed to take more fictitious particles by increasing the numbers of auxiliary masses, it is possible to obtain a trace-class operator under the additional conditions

$$\sum_j c_j\, m_j = \sum_j c_j\, m_j^3 = 0.$$

At least four auxiliary masses are then necessary. The terms which are not trace-class when only two fictitious particles are used, actually do *not* contribute to the final value of the energy functional $\mathcal{F}_{\rm PV}$ (their trace formally vanishes). For this reason, we have found more convenient to first take the $\mathbb{C}^4$–trace (which is enough to discard the problematic terms) and limit ourselves to two fictitious particles, as is usually done in the Physics literature. This suffices to provide a clear meaning to the energy.

The function M describes the linear response of the Dirac sea. It is well-known in the Physics literature [16, Eq. (5.39)]. We will see below that

$$\lim_{\Lambda\to\infty}\Big(\frac{2\log\Lambda}{3\pi}-M(k)\Big)=U(k):=\frac{|k|^2}{4\pi}\int_0^1\frac{z^2-z^4/3}{1+|k|^2(1-z^2)/4}\,dz. \quad (2.18)$$

The function in the right-hand side of (2.18) was first computed by Serber [37] and Uehling [44]. The same function U already appeared in our previous works dealing with pure electrostatic potentials [21, 18, 15]. This is a consequence of the gauge and relativistic invariances of full QED.

After having properly defined the functional $\mathcal{F}_{\rm PV}$, we need some of its differentiability properties. In this direction, we can prove the following

Theorem 2.2 (Differentiability of $\mathcal{F}_{\rm PV}$)**.** *Assume that c_j and m_j satisfy conditions* (2.10)*.*

(i) Let $\boldsymbol{A}\in\dot{H}^1_{\rm div}(\mathbb{R}^3)$ be such that 0 is not an eigenvalue of the operators $D_{m_j,\boldsymbol{A}}$ for $j=0,1,2$. Then the functional $\mathcal{F}_{\rm PV}$ is C^∞ in a neighborhood of $\boldsymbol{A}$.

(ii) The first derivative of $\mathcal{F}_{\rm PV}$ is given by

$$\langle \mathrm{d}\mathcal{F}_{\rm PV}(\boldsymbol{A}),(\mathfrak{v},\mathfrak{a})\rangle=\int_{\mathbb{R}^3}\big\langle(\rho_{\boldsymbol{A}},-j_{\boldsymbol{A}},),(\mathfrak{v},\mathfrak{a})\big\rangle_{\mathbb{R}^4}, \quad (2.19)$$

for all $(\mathfrak{v},\mathfrak{a})\in\dot{H}^1_{\rm div}(\mathbb{R}^3)$, where the density $\rho_{\boldsymbol{A}}$ and the current $j_{\boldsymbol{A}}$ are defined as

$$\rho_{\boldsymbol{A}}(x):=\big[\mathrm{tr}_{\mathbb{C}^4}\,Q_{\boldsymbol{A}}\big](x,x)\quad\text{and}\quad j_{\boldsymbol{A}}(x):=\big[\mathrm{tr}_{\mathbb{C}^4}\,\boldsymbol{\alpha}\,Q_{\boldsymbol{A}}\big](x,x), \quad (2.20)$$

and with $Q_{\boldsymbol{A}}$ refering to the kernel of the operator

$$Q_{\boldsymbol{A}}:=\sum_{j=0}^{2}c_j\,\mathbb{1}_{(-\infty,0)}\big(D_{m_j,\boldsymbol{A}}\big).$$

The operators $\mathrm{tr}_{\mathbb{C}^4}\,Q_{\boldsymbol{A}}$ and $\mathrm{tr}_{\mathbb{C}^4}\,\alpha_k Q_{\boldsymbol{A}}$ for $k=1,2,3$ are locally trace-class on $L^2(\mathbb{R}^3,\mathbb{C}^4)$, and $\rho_{\boldsymbol{A}}$ and $j_{\boldsymbol{A}}$ are well-defined functions in $L^1_{\rm loc}(\mathbb{R}^3)\cap\mathcal{C}$, where $\mathcal{C}$ is the Coulomb space

$$\mathcal{C}:=\Big\{f:\mathbb{R}^3\to\mathbb{C}:\int_{\mathbb{R}^3}\frac{|\widehat{f}(k)|^2}{|k|^2}\,dk<\infty\Big\}=\dot{H}^{-1}(\mathbb{R}^3). \quad (2.21)$$

(iii) There exists a universal constant $\eta>0$ such that the second derivative of $\mathcal{F}_{\rm PV}$ satisfies the estimate

$$\left\|\mathrm{d}^2\mathcal{F}_{\rm PV}(\boldsymbol{A})-\frac{1}{4\pi}\begin{pmatrix}-M&0\\0&M\end{pmatrix}\right\|\le 2K\Big(\sum_{j=0}^{2}\frac{|c_j|}{m_j}\Big)\|\boldsymbol{A}\|^2_{\dot{H}^1_{\rm div}(\mathbb{R}^3)} \quad (2.22)$$

for all $\boldsymbol{A}$ such that $\|\boldsymbol{A}\|_{\dot{H}^1_{\rm div}(\mathbb{R}^3)}\le\eta\sqrt{m_0}=\eta\sqrt{m}$.

Our estimate (2.22) means more precisely that

$$\left|\langle \boldsymbol{A}', \mathrm{d}^2\mathcal{F}_{\rm PV}(\boldsymbol{A})\,\boldsymbol{A}'\rangle - \frac{1}{4\pi}\int_{\mathbb{R}^3} M(k)\Big(\big|\widehat{B'}(k)\big|^2 - \big|\widehat{E'}(k)\big|^2\Big)\,dk\right| \leq 2K\left(\sum_{j=0}^{2}\frac{|c_j|}{m_j}\right)\|\boldsymbol{A}\|^2_{\dot H^1_{\rm div}(\mathbb{R}^3)}\|\boldsymbol{A}'\|^2_{\dot H^1_{\rm div}(\mathbb{R}^3)},$$

when $\boldsymbol{A}$ is small enough in $\dot H^1_{\rm div}(\mathbb{R}^3)$.

As a consequence of Lemma 2.1 and Theorem 2.2, we obtain

Corollary 2.1 (Regularity in a neighborhood of 0)**.** *There exists a positive radius η such that the functional $\mathcal{F}_{\rm PV}$ is $\mathcal{C}^\infty$ on the ball $\mathcal{B}(\eta) := \big\{\boldsymbol{A} \in \dot H^1_{\rm div}(\mathbb{R}^3) : \|\boldsymbol{A}\|_{\dot H^1_{\rm div}(\mathbb{R}^3)} < \eta\sqrt{m_0}\big\}$. On this ball, the differential $\mathrm{d}\mathcal{F}_{\rm PV}$ is given by* (2.19)*, whereas $\mathrm{d}^2\mathcal{F}_{\rm PV}$ satisfies estimate* (2.22)*.*

Proof. We fix η such that

$$C\eta < 1,$$

where C is the constant in statement *(iii)* of Lemma 2.1. For this choice, given any four-potential $\boldsymbol{A}$ in the ball $\mathcal{B}(\eta)$, 0 is not an eigenvalue of each of the operators $D_{m_j,\boldsymbol{A}}$. Corollary 2.1 then follows from Theorem 2.2. □

In the next sections, we explain how to use Theorems 2.1 and 2.2 in order to get the desired stability of the free Dirac vacuum, and to construct the polarized vacuum. We then come back to the proofs of Theorems 2.1 and 2.2 afterwards.

2.3. **Stability of the free Dirac vacuum.** Let $e > 0$ be the (bare) charge of the electron. Assume that $c_0 = 1$, and that c_j and m_j satisfy (2.7). We work under the condition that $e \leq \bar e$ for some fixed constant $\bar e$ (e is not allowed to be too large, but it can be arbitrarily small). All our constants will depend on $\bar e$, but not on e. Note that e is dimensionless here because we have already set the speed of light equal to 1. Using Theorem 2.1, we can properly define the Pauli-Villars Lagrangian in the absence of any external electromagnetic field, i.e. for $\boldsymbol{A}_{\rm ext} \equiv 0$, by

$$\boxed{\mathscr{L}^0_{\rm PV}(\boldsymbol{A}) := \mathcal{F}_{\rm PV}\big(e\boldsymbol{A}\big) + \frac{1}{8\pi}\int_{\mathbb{R}^3}\big(|B|^2 - |E|^2\big),}$$

on the Coulomb-gauge homogeneous Sobolev space $\dot H^1_{\rm div}(\mathbb{R}^3)$. The following result is a direct consequence of the properties of the functional $\mathcal{F}_2$ defined in (2.15), as well as on the regularity properties of $\mathcal{F}_{\rm PV}$.

Theorem 2.3 (Stability of the free Dirac vacuum)**.** *Assume that c_j and m_j satisfy* (2.10)*. The four-potential $\boldsymbol{A} \equiv 0$ is a saddle point of $\mathscr{L}^0_{\rm PV}$. It is the unique solution to the min-max problem*

$$\mathscr{L}^0_{\rm PV}(0,0) = \max_{\|\nabla V\|_{L^2} < \frac{r\sqrt{m_0}}{e}} \mathscr{L}^0_{\rm PV}(V,0) = \min_{\|\operatorname{curl} A\|_{L^2} < \frac{r\sqrt{m_0}}{e}} \mathscr{L}^0_{\rm PV}(0,A), \quad (2.23)$$

or, equivalently,

$$\begin{aligned}\mathscr{L}^0_{\mathrm{PV}}(0,0) &= \min_{\|\operatorname{curl} A\|_{L^2}<\frac{r\sqrt{m_0}}{e}} \ \sup_{\|\nabla V\|_{L^2}<\frac{r\sqrt{m_0}}{e}} \mathscr{L}^0_{\mathrm{PV}}(V,A) \\ &= \max_{\|\nabla V\|_{L^2}<\frac{r\sqrt{m_0}}{e}} \ \inf_{\|\operatorname{curl} A\|_{L^2}<\frac{r\sqrt{m_0}}{e}} \mathscr{L}^0_{\mathrm{PV}}(V,A),\end{aligned} \tag{2.24}$$

for some positive radius r which only depends on $\sum_{j=0}^{2}|c_j|(m_0/m_j)$ and $\bar{e}$ (the largest possible value of e).

As we have seen we can take the cut-off $\Lambda \to \infty$ which implies that $m_0/m_j \to 0$ for $j = 1, 2$, while keeping c_1 and c_2 bounded. We therefore see that the radius r of the ball of stability of the free vacuum does *not* depend on Λ if the bare parameters e and m_0 are kept fixed.

The electrostatic stability of the free Dirac vacuum was pointed out first by Chaix, Iracane and Lions [4, 5] and proved later in [1, 17, 18]. It is possible to include the exchange term and even establish the *global* stability of the free Dirac vacuum [17, 18, 19]. Dealing with magnetic fields is more complicated and, so far, we are only able to prove *local* stability, using the Pauli-Villars regularization. Because of lack of gauge symmetry, it is not clear whether the free Dirac sea is still stable under magnetic excitations when a sharp ultraviolet cut-off is used.

Proof. We choose $r > 0$ such that

$$r \leq \eta/\sqrt{2} \quad \text{and} \quad 2K\bigg(\sum_{j=0}^{2}\frac{|c_j|}{m_j}\bigg)m_0\big(r^2+2m_0r^4\big) \leq \frac{1}{8\pi\bar{e}^2}, \tag{2.25}$$

where K is the constant appearing in (2.14), and where η is the constant in statement (iii) of Theorem 2.2. We recall that $e \leq \bar{e}$. Consider now any $\boldsymbol{A}$ such that $\|\nabla V\|_{L^2} \leq r\sqrt{m_0}/e$ and $\|\operatorname{curl} A\|_{L^2} \leq r\sqrt{m_0}/e$ (which implies $\|\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} = \|\boldsymbol{F}\|_{L^2} \leq \sqrt{2m_0}r/e$). By (2.14), we have

$$\begin{aligned}\big|\mathcal{F}_{\mathrm{PV}}(e\boldsymbol{A}) - \mathcal{F}_2(e\boldsymbol{F})\big| &\leq K\bigg(\bigg(\sum_{j=0}^{2}\frac{|c_j|}{m_j}\bigg)e^4\|\boldsymbol{F}\|_{L^2}^4 + \bigg(\sum_{j=0}^{2}\frac{|c_j|}{m_j^2}\bigg)e^6\|\boldsymbol{F}\|_{L^2}^6\bigg) \\ &\leq 2K\bigg(\sum_{j=0}^{2}\frac{|c_j|}{m_j}\bigg)m_0\big(r^2+2m_0r^4\big)e^2\|\boldsymbol{F}\|_{L^2}^2 \\ &\leq \frac{1}{8\pi}\|\boldsymbol{F}\|_{L^2}^2.\end{aligned} \tag{2.26}$$

Using Formula (2.15) for $\mathcal{F}_2$, we get

$$\mathscr{L}^0_{\mathrm{PV}}(0,A) \geq \frac{e^2}{8\pi}\int_{\mathbb{R}^3} M(k)|\widehat{B}(k)|^2\,dk \geq 0,$$

with equality if and only $A \equiv 0$, since $M > 0$. Similarly,

$$\mathscr{L}^0_{\mathrm{PV}}(V,0) \leq -\frac{e^2}{8\pi}\int_{\mathbb{R}^3} M(k)|\widehat{E}(k)|^2\,dk \leq 0,$$

with equality if and only $V \equiv 0$. Thus we have shown (2.23). The equivalence between (2.23) and (2.24) is a classical fact of convex analysis, see [9, Prop. 1.2, Chap. VI].

Finally, since we can deduce from (2.22) that

$$\left\| \mathrm{d}^2 \mathscr{L}^0_{\mathrm{PV}}(\boldsymbol{A}) - \frac{1}{4\pi} \begin{pmatrix} -1-e^2M & 0 \\ 0 & 1+e^2M \end{pmatrix} \right\| \leq 2Ke^2 \Big(\sum_{j=0}^{2} \frac{|c_j|}{m_j} \Big) \|\boldsymbol{F}\|_{L^2}^2 \leq 4Km_0 \Big(\sum_{j=0}^{2} \frac{|c_j|}{m_j} \Big) r^2,$$

for $e\|\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \leq r\sqrt{2m_0} \leq \eta\sqrt{m_0}$, we deduce that $\mathscr{L}^0_{\mathrm{PV}}$ is strictly convex with respect to A and strictly concave with respect to V, provided that r satisfies the additional condition

$$4Km_0 \Big(\sum_{j=0}^{2} \frac{|c_j|}{m_j} \Big) r^2 < \frac{1}{4\pi}. \tag{2.27}$$

This implies uniqueness of the saddle point by [9, Prop 1.5, Chap. VI]. □

2.4. **Polarized Dirac vacuum in external electromagnetic fields.** Finally, we include an external electromagnetic field $\boldsymbol{A}_{\mathrm{ext}}$ and we look for the corresponding stable polarized Dirac vacuum, which is a stationary state of the Pauli-Villars Lagrangian functional

$$\boxed{\mathscr{L}^{\boldsymbol{A}_{\mathrm{ext}}}_{\mathrm{PV}}(\boldsymbol{A}) := \mathcal{F}_{\mathrm{PV}}\big(e(\boldsymbol{A}+\boldsymbol{A}_{\mathrm{ext}})\big) + \frac{1}{8\pi}\int_{\mathbb{R}^3} \big(|B|^2 - |E|^2\big),}$$

in $\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$. Our main result is

Theorem 2.4 (Existence of the polarized vacuum in small external fields)**.** *Assume that c_j and m_j satisfy* (2.10)*. Let r be the same constant as in Theorem 2.3.*

(i) For any

$$e\|\boldsymbol{A}_{\mathrm{ext}}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} < \frac{r\sqrt{m_0}}{8}, \tag{2.28}$$

there exists a unique solution $\boldsymbol{A}_* = (V_*, A_*) \in \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$ to the min-max problem

$$\mathscr{L}^{\boldsymbol{A}_{\mathrm{ext}}}_{\mathrm{PV}}(\boldsymbol{A}_*) = \max_{\|\nabla V\|_{L^2} < \frac{r\sqrt{m_0}}{4e}} \mathscr{L}^{\boldsymbol{A}_{\mathrm{ext}}}_{\mathrm{PV}}(V, A_*) = \min_{\|\operatorname{curl} A\|_{L^2} < \frac{r\sqrt{m_0}}{4e}} \mathscr{L}^{\boldsymbol{A}_{\mathrm{ext}}}_{\mathrm{PV}}(V_*, A),$$

or, equivalently, to

$$\begin{aligned} \mathscr{L}^{\boldsymbol{A}_{\mathrm{ext}}}_{\mathrm{PV}}(\boldsymbol{A}_*) &= \max_{\|\nabla V\|_{L^2} < \frac{r\sqrt{m_0}}{4e}} \ \inf_{\|\operatorname{curl} A\|_{L^2} < \frac{r\sqrt{m_0}}{4e}} \mathscr{L}^{\boldsymbol{A}_{\mathrm{ext}}}_{\mathrm{PV}}(\boldsymbol{A}) \\ &= \min_{\|\operatorname{curl} A\|_{L^2} < \frac{r\sqrt{m_0}}{4e}} \ \sup_{\|\nabla V\|_{L^2} < \frac{r\sqrt{m_0}}{4e}} \mathscr{L}^{\boldsymbol{A}_{\mathrm{ext}}}_{\mathrm{PV}}(\boldsymbol{A}). \end{aligned} \tag{2.29}$$

(ii) The four-potential $\boldsymbol{A}_*$ is a solution to the nonlinear equations

$$\begin{cases} -\Delta V_* = 4\pi e\, \rho_{\boldsymbol{A}_* + \boldsymbol{A}_{\mathrm{ext}}}, \\ -\Delta A_* = 4\pi e\, j_{\boldsymbol{A}_* + \boldsymbol{A}_{\mathrm{ext}}}, \end{cases} \tag{2.30}$$

where $\rho_{\boldsymbol{A}_*+\boldsymbol{A}_{\rm ext}}$ and $j_{\boldsymbol{A}_*+\boldsymbol{A}_{\rm ext}}$ refer to the charge and current densities defined in Theorem 2.2, that is, associated with the operator

$$Q_* = \sum_{j=0}^{2} c_j \, \mathbb{1}_{(-\infty,0)}\big(D_{m_j,e(\boldsymbol{A}_*+\boldsymbol{A}_{\rm ext})}\big). \tag{2.31}$$

Solutions to the self-consistent equation (2.30) have been constructed in the previous works [17, 18, 20], with a sharp ultraviolet cut-off and including the exchange term, but in the purely electrostatic case $A_{\rm ext} = A_* = 0$. In this special case it is possible to obtain the polarized vacuum as a *global* minimizer. The method of [17, 18, 20] does not seem to be applicable with magnetic fields, however. To our knowledge, Theorem 2.4 is the first result dealing with self-consistent magnetic fields in the Hartree-Fock approximation of QED.

Equations (2.30) and (2.31) are well known in the Physics literature (see, e.g., [10, Eq. (62)–(64)]). In Relativistic Density Functional Theory, the exchange term is replaced by an effective functional of the density, which leads to formally similar equations.

The proof of Theorem 2.4 is based on tools of convex analysis, using that $\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}$ has the local saddle point geometry by Theorem 2.1.

Proof. Let us define the balls

$$\mathcal{B}_{\rm V}(r) := \big\{V \in L^6(\mathbb{R}^3,\mathbb{R}) \ : \ e\|\nabla V\|_{L^2} \leq r\sqrt{m_0}\big\},$$

and

$$\mathcal{B}_{\rm A}(r) := \big\{A \in L^6(\mathbb{R}^3,\mathbb{R}^3) \ : \ e\|\operatorname{curl} A\|_{L^2} \leq r\sqrt{m_0}\big\}.$$

As we have already shown in the proof of Theorem 2.3, when r satisfies condition (2.25), the function $\boldsymbol{A} \mapsto \mathscr{L}_{\rm PV}^0(\boldsymbol{A})$ is strictly convex with respect to A and strictly concave with respect to V on $\mathcal{B}_{\rm V}(r) \times \mathcal{B}_{\rm A}(r)$.

We now assume that the external field $\boldsymbol{A}_{\rm ext} \in \mathcal{B}_{\rm V}(\varepsilon r) \times \mathcal{B}_{\rm A}(\varepsilon r)$ for some $\varepsilon < 1/3$ to be chosen later. Then $\boldsymbol{A} + \boldsymbol{A}_{\rm ext}$ is in $\mathcal{B}_{\rm V}(r) \times \mathcal{B}_{\rm A}(r)$ for all $\boldsymbol{A} \in \mathcal{B}_{\rm V}(2\varepsilon r) \times \mathcal{B}_{\rm A}(2\varepsilon r)$. Therefore, $\boldsymbol{A} \mapsto \mathscr{L}_{\rm PV}^0(\boldsymbol{A} + \boldsymbol{A}_{\rm ext})$ is also strictly convex with respect to A and strictly concave with respect to V on $\mathcal{B}_{\rm V}(2\varepsilon r)\times$ $\mathcal{B}_{\rm A}(2\varepsilon r)$. Now we remark that

$$\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(\boldsymbol{A}) = \mathscr{L}_{\rm PV}^0(\boldsymbol{A}+\boldsymbol{A}_{\rm ext}) + \frac{1}{8\pi}\int_{\mathbb{R}^3} \big(2E\cdot E_{\rm ext} - 2B\cdot B_{\rm ext} + |E_{\rm ext}|^2 - |B_{\rm ext}|^2\big),$$

which shows that $\boldsymbol{A} \mapsto \mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(\boldsymbol{A})$ has the same convexity and concavity properties on $\mathcal{B}_{\rm V}(2\varepsilon r) \times \mathcal{B}_{\rm A}(2\varepsilon r)$.

Since $\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}$ is strongly continuous on $\mathcal{B}_{\rm V}(2\varepsilon r)\times\mathcal{B}_{\rm A}(2\varepsilon r)$ by Theorem 2.1, a classical result from convex analysis implies that $\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}$ possesses at least one saddle point $\boldsymbol{A}_* = (V_*, A_*) \in \mathcal{B}_{\rm V}(2\varepsilon r) \times \mathcal{B}_{\rm A}(2\varepsilon r)$, solving

$$\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(\boldsymbol{A}_*) = \max_{V\in\mathcal{B}_V(2\varepsilon r)} \mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(V, A_*) = \min_{A\in\mathcal{B}_A(2\varepsilon r)} \mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(V_*, A).$$

See for instance [9, Prop. 2.1, Chap. VI]. Uniqueness follows from the strict concavity and convexity, by [9, Prop 1.5, Chap. VI].

It only remains to verify that $\boldsymbol{A}_*$ does not lie on the boundary of $\mathcal{B}_{\rm V}(2\varepsilon r)\times \mathcal{B}_{\rm A}(2\varepsilon r)$. Similarly as in (2.26), we first compute

$$\begin{aligned}\left|\mathcal{F}_{\rm PV}(e\boldsymbol{A}')-\mathcal{F}_2(e\boldsymbol{F}')\right| &\leq K\bigg(\sum_{j=0}^{2}\frac{|c_j|}{m_j}\bigg)\bigg(e^4\|\boldsymbol{F}'\|_{L^2}^4+\frac{e^6}{m_0}\|\boldsymbol{F}'\|_{L^2}^6\bigg)\\ &\leq \frac{9\,\varepsilon^2}{8\pi}\|\boldsymbol{F}'\|_{L^2}^2,\end{aligned} \tag{2.32}$$

for all $\boldsymbol{A}'\in\mathcal{B}_{\rm V}(3\varepsilon r)\times\mathcal{B}_{\rm A}(3\varepsilon r)$, when r satisfies (2.25) and $\varepsilon<1/3$. Using that $\boldsymbol{A}+\boldsymbol{A}_{\rm ext}\in\mathcal{B}_{\rm V}(3\varepsilon r)\times\mathcal{B}_{\rm A}(3\varepsilon r)$, we obtain

$$\begin{aligned}&\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(V,A)-\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(V,-A_{\rm ext})\\ &\geq e^2\mathcal{F}_2(0,B+B_{\rm ext})+\frac{1}{8\pi}\int_{\mathbb{R}^3}|\operatorname{curl}A|^2-\frac{1}{8\pi}\int_{\mathbb{R}^3}|\operatorname{curl}A_{\rm ext}|^2-\frac{81\,\varepsilon^4r^2m_0}{4\pi e^2}\\ &\geq \frac{1}{8\pi}\int_{\mathbb{R}^3}|\operatorname{curl}A|^2-\frac{\varepsilon^2r^2m_0(162\,\varepsilon^2+1)}{8\pi e^2},\end{aligned}$$

since $\mathcal{F}_2$ is a non-negative functional. When A belongs to the boundary of $\mathcal{B}_A(2\varepsilon r)$, we obtain

$$\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(V,A)\geq\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(V,-A_{\rm ext})+\frac{3\varepsilon^2r^2}{8\pi}\big(1-54\varepsilon^2\big)m_0.$$

Choosing for instance $\varepsilon=1/8$, the right-hand side is positive, so that

$$e^2\int_{\mathbb{R}^3}|\operatorname{curl}A_*|^2<4\varepsilon^2r^2m_0,$$

otherwise we would have $\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(V_*,A_*)>\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(V_*,-A_{\rm ext})$, which contradicts the fact that A_* minimizes $A\mapsto\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(V_*,A)$. Similarly, we have

$$\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(V,A)-\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}(-V_{\rm ext},A)\leq-\frac{1}{8\pi}\int_{\mathbb{R}^3}|\nabla V|^2+\frac{\varepsilon^2r^2m_0(162\,\varepsilon^2+1)}{8\pi e^2}, \tag{2.33}$$

which can be used to show that

$$e^2\int_{\mathbb{R}^3}|\nabla V_*|^2<4\varepsilon^2r^2m_0.$$

The unique saddle point $\boldsymbol{A}_*=(V_*,A_*)$ being in the interior of the set $\mathcal{B}_{\rm V}(2\varepsilon r)\times\mathcal{B}_{\rm A}(2\varepsilon r)$, the derivative of $\mathscr{L}_{\rm PV}^{\boldsymbol{A}_{\rm ext}}$ must vanish at this point. The self-consistent equation (2.30) follows from Theorem 2.2. □

The rest of the paper is devoted to the proofs of Theorems 2.1 and 2.2. Our strategy is as follows. First, in Section 3, we show that the functional $\mathcal{F}_{\rm PV}$ is well-defined for four-potentials $\boldsymbol{A}$ with an appropriate decay in x-space (the integrability of $\boldsymbol{A}$ on $\mathbb{R}^3$ is enough). Then, we compute things more precisely in Section 4, and we exhibit the cancellations which show that this functional can be uniquely extended by continuity to $\dot{H}^1_{\rm div}(\mathbb{R}^3)$.

3. Proper definition of the Pauli-Villars functional for potentials with fast decay

The purpose of this section is to prove that the operator

$$\operatorname{tr}_{\mathbb{C}^4} T_{\boldsymbol{A}} := \frac{1}{2}\sum_{j=0}^{2} c_j \operatorname{tr}_{\mathbb{C}^4}\left(|D_{m_j,0}| - |D_{m_j,\boldsymbol{A}}|\right), \tag{3.1}$$

is trace-class, when the four-potential $\boldsymbol{A} := (V, A)$ decays sufficiently fast. The proof relies on an expansion of $\mathcal{F}_{\mathrm{PV}}(\boldsymbol{A})$ with respect to the four-potential $\boldsymbol{A}$ using the resolvent formula, but for which we actually do *not* need that $\boldsymbol{A}$ is small. Our precise statement is the following

Proposition 3.1 ($\operatorname{tr}_{\mathbb{C}^4} T_{\boldsymbol{A}}$ is in $\mathfrak{S}_1$)**.** *Assume that c_j and m_j satisfy conditions* (2.10)*. Then, the operator $\operatorname{tr}_{\mathbb{C}^4} T_{\boldsymbol{A}}$ is trace-class whenever $\boldsymbol{A} \in L^1(\mathbb{R}^3,\mathbb{R}^4) \cap H^1(\mathbb{R}^3,\mathbb{R}^4)$.*

Remark 3.1. For this result, it is not important that $\operatorname{div} A = 0$, hence we do not require that $A \in \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$.

The rest of this section is devoted to the proof of Proposition 3.1.

Proof. Our starting point is the integral formula

$$|x| = \frac{1}{\pi}\int_{\mathbb{R}} \frac{x^2}{x^2+\omega^2}\,d\omega = \frac{1}{2\pi}\int_{\mathbb{R}} \left(2 - \frac{i\omega}{x+i\omega} + \frac{i\omega}{x-i\omega}\right) d\omega. \tag{3.2}$$

When T is a self-adjoint operator on $L^2(\mathbb{R}^3,\mathbb{R}^4)$, with domain $D(T)$, it follows from (3.2) using standard functional calculus (see e.g. [31]), that the absolute value $|T|$ of T is given by

$$|T| = \frac{1}{2\pi}\int_{\mathbb{R}} \left(2 - \frac{i\omega}{T+i\omega} + \frac{i\omega}{T-i\omega}\right) d\omega. \tag{3.3}$$

Let us remark that this integral is convergent when seen as an operator from $D(T^2)$ to the ambient Hilbert space. In particular,

$$\left\| \frac{T^2}{T^2+\omega^2} \right\|_{D(T^2)\to L^2(\mathbb{R}^3,\mathbb{C}^4)} \leq \min\left\{1, \omega^{-2}\left\|T^2\right\|_{D(T^2)\to L^2(\mathbb{R}^3,\mathbb{C}^4)}\right\}.$$

Since the domains of $D^2_{m_j,0}$ and $D^2_{m_j,\boldsymbol{A}}$ are both equal to $H^2(\mathbb{R}^3,\mathbb{C}^4)$, we deduce that we can write

$$\begin{aligned} T_{\boldsymbol{A}} = \frac{1}{4\pi}\int_{\mathbb{R}} \sum_{j=0}^{2} c_j \Big(&\frac{i\omega}{D_{m_j,\boldsymbol{A}}+i\omega} - \frac{i\omega}{D_{m_j,\boldsymbol{A}}-i\omega} \\ &- \frac{i\omega}{D_{m_j,0}+i\omega} + \frac{i\omega}{D_{m_j,0}-i\omega}\Big)\, d\omega \end{aligned} \tag{3.4}$$

on $H^2(\mathbb{R}^3,\mathbb{C}^4)$. Here and everywhere else it is not a problem if $D_{m_j,\boldsymbol{A}}$ has 0 as an eigenvalue. The operator $D_{m_j,\boldsymbol{A}} + i\omega$ is invertible for $\omega \neq 0$, and $(i\omega)(D_{m_j,\boldsymbol{A}} + i\omega)^{-1}$ stays uniformly bounded in the limit $\omega \to 0$.

In order to establish Proposition 3.1, we will prove that the $\mathbb{C}^4$–trace of the integral in the right-hand side of (3.4) defines a trace-class operator

according to the inequality

$$\int_{\mathbb{R}} \Big\| \sum_{j=0}^{2} c_j \ \mathrm{tr}_{\mathbb{C}^4} \Big(\frac{i\omega}{D_{m_j,\boldsymbol{A}} + i\omega} - \frac{i\omega}{D_{m_j,\boldsymbol{A}} - i\omega} - \frac{i\omega}{D_{m_j,0} + i\omega} + \frac{i\omega}{D_{m_j,0} - i\omega} \Big) \Big\|_{\mathfrak{S}_1} d\omega < \infty, \quad (3.5)$$

which we can establish when $\boldsymbol{A} \in L^1(\mathbb{R}^3, \mathbb{R}^4) \cap H^1(\mathbb{R}^3, \mathbb{R}^4)$. This will complete the proof of Proposition 3.1.

As a consequence, our task reduces to derive estimates in Schatten spaces on the integrand operator

$$\mathcal{R}(\omega, \boldsymbol{A}) := \sum_{j=0}^{2} c_j \ \mathrm{tr}_{\mathbb{C}^4} \Big(\frac{i\omega}{D_{m_j,\boldsymbol{A}} + i\omega} - \frac{i\omega}{D_{m_j,\boldsymbol{A}} - i\omega} - \frac{i\omega}{D_{m_j,0} + i\omega} + \frac{i\omega}{D_{m_j,0} - i\omega} \Big),$$

which we can integrate with respect to ω. To this end, we use the resolvent expansion, truncated at the sixth order,

$$\begin{aligned} \frac{i\omega}{D_{m_j,\boldsymbol{A}} + i\omega} - \frac{i\omega}{D_{m_j,0} + i\omega} &= \sum_{n=1}^{5} \frac{i\omega}{D_{m_j,0} + i\omega} \Big((\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big)^n \\ &\quad + \frac{i\omega}{D_{m_j,\boldsymbol{A}} + i\omega} \Big((\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big)^6, \end{aligned} \quad (3.6)$$

and the similar expression for the term with $-i\omega$ instead of $+i\omega$. Again, we insist on the fact that this expansion makes perfect sense for $\omega \neq 0$, even if the spectrum of $D_{m_j,\boldsymbol{A}}$ contains 0. This allows us to write

$$\begin{aligned} \mathcal{R}(\omega, \boldsymbol{A}) = \sum_{n=1}^{5} \mathrm{tr}_{\mathbb{C}^4} \Big(R_n(\omega, \boldsymbol{A}) + R_n(-\omega, \boldsymbol{A}) \Big) \\ + \mathrm{tr}_{\mathbb{C}^4} \big(R'_6(\omega, \boldsymbol{A}) + R'_6(-\omega, \boldsymbol{A}) \big), \end{aligned} \quad (3.7)$$

with

$$R_n(\omega, \boldsymbol{A}) := \sum_{j=0}^{2} c_j \frac{i\omega}{D_{m_j,0} + i\omega} \Big((\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big)^n, \quad (3.8)$$

and

$$R'_6(\omega, \boldsymbol{A}) := \sum_{j=0}^{2} c_j \frac{i\omega}{D_{m_j,\boldsymbol{A}} + i\omega} \Big((\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big)^6. \quad (3.9)$$

Our purpose is to prove that

$$\int_{\mathbb{R}} \Big(\sum_{n=1}^{5} \big\| \mathrm{tr}_{\mathbb{C}^4} \big(R_n(\omega, \boldsymbol{A}) + R_n(-\omega, \boldsymbol{A}) \big) \big\|_{\mathfrak{S}_1} + \big\| \mathrm{tr}_{\mathbb{C}^4} \big(R'_6(\omega, \boldsymbol{A}) + R'_6(-\omega, \boldsymbol{A}) \big) \big\|_{\mathfrak{S}_1} \Big) d\omega < \infty. \quad (3.10)$$

Estimate on the sixth order term. We first estimate the sixth order term $R_6'(\omega, \boldsymbol{A})$ in (3.7) which is the simplest one. The $\mathbb{C}^4$–trace is not going to be helpful for us here. First we use the inequality

$$\Big\| \frac{i\omega}{D_{m_j,\boldsymbol{A}} + i\omega} \Big\| \leq 1,$$

which, in particular, takes care of the possibility of having 0 in the spectrum of $D_{m_j,\boldsymbol{A}}$. Combining with Hölder's inequality in Schatten spaces, we obtain

$$\begin{aligned} \Big\| \frac{i\omega}{D_{m_j,\boldsymbol{A}} + i\omega} \Big((\boldsymbol{\alpha}\cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big)^6 \Big\|_{\mathfrak{S}_1} \\ \leq \Big\| (\boldsymbol{\alpha}\cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big\|_{\mathfrak{S}_6}^6. \end{aligned} \tag{3.11}$$

We next use the Kato-Seiler-Simon inequality (2.5), similarly as in the proof of Lemma 2.1, which gives us

$$\forall p > 3, \ \Big\| (\boldsymbol{\alpha}\cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big\|_{\mathfrak{S}_p} \leq (I_p)^{\frac{1}{p}} (m_j^2 + \omega^2)^{\frac{3}{2p} - \frac{1}{2}} \big\| \boldsymbol{A} \big\|_{L^p},$$

where

$$I_p := \frac{1}{2\pi^2} \int_0^\infty \frac{r^2\, dr}{(1+r^2)^{\frac{p}{2}}}.$$

For $p = 6$, we can use the Sobolev inequalities

$$\|V\|_{L^6} \leq S \|\nabla V\|_{L^2} \quad \text{and} \quad \|A\|_{L^6} \leq S \|\nabla A\|_{L^2}, \tag{3.12}$$

to obtain an estimate in terms of the gradient $\nabla \boldsymbol{A}$ by

$$\Big\| (\boldsymbol{\alpha}\cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big\|_{\mathfrak{S}_6} \leq \frac{(I_6)^{\frac{1}{6}} S}{(m_j^2 + \omega^2)^{\frac{1}{4}}} \big\| \nabla \boldsymbol{A} \big\|_{L^2}.$$

Inserting in (3.11), we have

$$\big\| R_6'(\omega, \boldsymbol{A}) \big\|_{\mathfrak{S}_1} \leq \sum_{j=0}^{2} |c_j| \, \frac{S^6 I_6}{(m_j^2 + \omega^2)^{\frac{3}{2}}} \, \big\| \nabla \boldsymbol{A} \big\|_{L^2}^6, \tag{3.13}$$

so that

$$\int_{\mathbb{R}} \|R_6'(\omega, \boldsymbol{A})\|_{\mathfrak{S}_1} \, d\omega \leq S^6 I_6 \Big(\sum_{j=0}^{2} \frac{|c_j|}{m_j^2} \Big) \|\nabla \boldsymbol{A}\|_{L^2}^6 \int_{\mathbb{R}} \frac{d\omega}{(1+\omega^2)^{\frac{3}{2}}}. \tag{3.14}$$

The term with $+i\omega$ replaced by $-i\omega$ is treated similarly.

Estimate on the fifth order term. The method that we have used for the sixth order term of (3.6) can be applied in a similar fashion to the fifth order term, leading to the estimate

$$\int_{\mathbb{R}} \|R_5(\pm\omega, \boldsymbol{A})\|_{\mathfrak{S}_1} d\omega \leq I_5 \Big(\sum_{j=0}^{2} \frac{|c_j|}{m_j} \Big) \|\boldsymbol{A}\|_{L^5}^5 \int_{\mathbb{R}} \frac{|\omega|\, d\omega}{(1+\omega^2)^{\frac{3}{2}}}. \tag{3.15}$$

None of these estimates use simplifications coming from the $\mathbb{C}^4$–trace. The latter is only useful for lower order terms.

Estimate on the fourth order term. For the other terms in (3.6), we need more precise estimates based on conditions (2.8) satisfied by the coefficients c_j and the masses m_j. We start by considering the fourth order term, for which we use the identity $c_0 + c_1 + c_2 = 0$ to write

$$\begin{aligned} R_4(\omega, \boldsymbol{A}) = &\sum_{j=0}^{2} c_j \sum_{k=0}^{4} \Big(\frac{1}{D_{m_0,0} + i\omega} \big(\boldsymbol{\alpha} \cdot A - V \big) \Big)^k \times \\ &\times \Big(\frac{i\omega}{D_{m_j,0} + i\omega} - \frac{i\omega}{D_{m_0,0} + i\omega} \Big) \Big(\big(\boldsymbol{\alpha} \cdot A - V \big) \frac{1}{D_{m_j,0} + i\omega} \Big)^{4-k}. \end{aligned}$$

Next we use that

$$\begin{aligned} \Big\| \frac{i\omega}{D_{m_j,0} + i\omega} - \frac{i\omega}{D_{m_0,0} + i\omega} \Big\| = &\Big\| \frac{m_0 - m_j}{D_{m_j,0} + i\omega} \boldsymbol{\beta} \frac{i\omega}{D_{m_0,0} + i\omega} \Big\| \\ \leq &\big(m_j - m_0 \big) \frac{|\omega|}{m_0^2 + \omega^2}, \end{aligned} \tag{3.16}$$

since $m_j \geq m_0$, and we argue as before, using this time $\boldsymbol{A} \in L^4(\mathbb{R}^3, \mathbb{R}^4)$. We obtain

$$\big\| R_4(\pm\omega, \boldsymbol{A}) \big\|_{\mathfrak{S}_1} \leq \frac{5 I_4 |\omega|}{(m_0^2 + \omega^2)^{\frac{3}{2}}} \sum_{j=0}^{2} |c_j| \left(m_j - m_0 \right) \|\boldsymbol{A}\|_{L^4}^4, \tag{3.17}$$

hence

$$\int_{\mathbb{R}} \big\| R_4(\pm\omega, \boldsymbol{A}) \big\|_{\mathfrak{S}_1} \, d\omega \leq 5 I_4 \|\boldsymbol{A}\|_{L^4}^4 \sum_{j=0}^{2} |c_j| \, \frac{m_j - m_0}{m_0} \int_{\mathbb{R}} \frac{|\omega| \, d\omega}{(1 + \omega^2)^{\frac{3}{2}}}. \tag{3.18}$$

Notice again that we have not used the $\mathbb{C}^4$–trace in our estimate of the fourth order term.

Estimate on the first order term. In order to deal with the first, second and third order terms, we need to use more cancellations. We start by considering the first order term for which we can write

$$\begin{aligned} &\frac{i\omega}{D_{m_j,0} + i\omega} \big(\boldsymbol{\alpha} \cdot A - V \big) \frac{1}{D_{m_j,0} + i\omega} - \frac{i\omega}{D_{m_j,0} - i\omega} \big(\boldsymbol{\alpha} \cdot A - V \big) \frac{1}{D_{m_j,0} - i\omega} \\ = &\frac{2\omega^2}{D_{m_j,0}^2 + \omega^2} \big(\boldsymbol{\alpha} \cdot A - V \big) \frac{1}{D_{m_j,0} + i\omega} + \frac{1}{D_{m_j,0} - i\omega} \big(\boldsymbol{\alpha} \cdot A - V \big) \frac{2\omega^2}{D_{m_j,0}^2 + \omega^2}. \end{aligned}$$

Inserting

$$\frac{1}{D_{m_j,0} \pm i\omega} = \frac{D_{m_j,0} \mp i\omega}{D_{m_j,0}^2 + \omega^2}, \tag{3.19}$$

we obtain

$$\begin{aligned} &\frac{i\omega}{D_{m_j,0} + i\omega} \big(\boldsymbol{\alpha} \cdot A - V \big) \frac{1}{D_{m_j,0} + i\omega} - \frac{i\omega}{D_{m_j,0} - i\omega} \big(\boldsymbol{\alpha} \cdot A - V \big) \frac{1}{D_{m_j,0} - i\omega} \\ &\qquad = \frac{2\omega^2}{D_{m_j,0}^2 + \omega^2} \big\{ \boldsymbol{\alpha} \cdot A - V, D_{m_j,0} \big\} \frac{1}{D_{m_j,0}^2 + \omega^2}, \end{aligned}$$

where the notation $\{T_1, T_2\}$ refers to the anti-commutator operator

$$\{T_1, T_2\} := T_1 T_2 + T_2 T_1.$$

At this stage, we recall that

$$\big(\boldsymbol{\alpha}\cdot X\big)\big(\boldsymbol{\alpha}\cdot Y\big) = X\cdot Y + i(X\times Y)\cdot\boldsymbol{\Sigma}, \tag{3.20}$$

for all $(X,Y)\in(\mathbb{R}^3)^2$. In this formula, $X\times Y$ is the cross product of the vectors X and Y, whereas the notation $\boldsymbol{\Sigma}=(\boldsymbol{\Sigma}_1,\boldsymbol{\Sigma}_2,\boldsymbol{\Sigma}_3)$ refers to the matrices

$$\boldsymbol{\Sigma}_j := \begin{pmatrix}\boldsymbol{\sigma}_j & 0\\ 0 & \boldsymbol{\sigma}_j\end{pmatrix}. \tag{3.21}$$

As a consequence, we obtain

$$\big\{\boldsymbol{\alpha}\cdot p, \boldsymbol{\alpha}\cdot A\big\} = \big\{p,A\big\}_{\mathbb{R}^3} + i\big(p\times A + A\times p\big)\cdot\boldsymbol{\Sigma} = \big\{p,A\big\}_{\mathbb{R}^3} + B\cdot\boldsymbol{\Sigma},$$

where $\{\cdot,\cdot\}_{\mathbb{R}^3}$ is a notation for

$$\big\{S,T\big\}_{\mathbb{R}^3} := S\cdot T + T\cdot S.$$

Since $\boldsymbol{\beta}\boldsymbol{\alpha}_k+\boldsymbol{\alpha}_k\boldsymbol{\beta}=0$, we deduce that

$$\big\{\boldsymbol{\alpha}\cdot A - V, D_{m_j,0}\big\} = \big\{p, A-V\boldsymbol{\alpha}\big\}_{\mathbb{R}^3} + B\cdot\boldsymbol{\Sigma} - 2m_jV\boldsymbol{\beta}. \tag{3.22}$$

This finally gives us

$$R_1(\omega,\boldsymbol{A}) + R_1(-\omega,\boldsymbol{A}) = 2\omega^2\big(\mathcal{R}_{1,1}+\mathcal{R}_{1,2}\big), \tag{3.23}$$

where

$$\mathcal{R}_{1,1} := \sum_{j=0}^{2} c_j\,\frac{1}{p^2+m_j^2+\omega^2}\Big(\big\{p,A-V\boldsymbol{\alpha}\big\}_{\mathbb{R}^3}+B\cdot\boldsymbol{\Sigma}\Big)\frac{1}{p^2+m_j^2+\omega^2}, \tag{3.24}$$

and

$$\mathcal{R}_{1,2} := -2\sum_{j=0}^{2} c_jm_j\,\frac{1}{p^2+m_j^2+\omega^2}\,V\boldsymbol{\beta}\,\frac{1}{p^2+m_j^2+\omega^2}. \tag{3.25}$$

Concerning the operator $\mathcal{R}_{1,1}$, the last step consists in using identities (2.7) and the two expansions

$$\begin{aligned}\frac{1}{p^2+m_j^2+\omega^2} &= \frac{1}{p^2+m_0^2+\omega^2} + \frac{m_0^2-m_j^2}{(p^2+m_0^2+\omega^2)(p^2+m_j^2+\omega^2)}\\ &= \frac{1}{p^2+m_0^2+\omega^2} + \frac{m_0^2-m_j^2}{(p^2+m_0^2+\omega^2)^2}\\ &\qquad + \frac{(m_0^2-m_j^2)^2}{(p^2+m_j^2+\omega^2)(p^2+m_0^2+\omega^2)^2}.\end{aligned} \tag{3.26}$$

This gives

$$\begin{aligned}\mathcal{R}_{1,1} = \sum_{j=0}^{2} c_j(m_0^2-m_j^2)^2\Bigg(&\\ \frac{1}{(p^2+m_0^2+\omega^2)^2}(\{p,A-V\boldsymbol{\alpha}\}_{\mathbb{R}^3}+B\cdot\boldsymbol{\Sigma})\frac{1}{(p^2+m_0^2+\omega^2)(p^2+m_j^2+\omega^2)}&\\ +\frac{1}{(p^2+m_j^2+\omega^2)(p^2+m_0^2+\omega^2)^2}(\{p,A-V\boldsymbol{\alpha}\}_{\mathbb{R}^3}+B\cdot\boldsymbol{\Sigma})\frac{1}{p^2+m_j^2+\omega^2}&\\ +\frac{1}{p^2+m_0^2+\omega^2}(\{p,A-V\boldsymbol{\alpha}\}_{\mathbb{R}^3}+B\cdot\boldsymbol{\Sigma})\frac{1}{(p^2+m_j^2+\omega^2)(p^2+m_0^2+\omega^2)^2}\Bigg).&\end{aligned}$$

We now use the fact that $\boldsymbol{A} \in L^1(\mathbb{R}^3, \mathbb{R}^4)$, $B = i(p \times A + A \times p)$, as well as the Kato-Seiler-Simon inequality (2.5) to get

$$\big\|\mathcal{R}_{1,1}\big\|_{\mathfrak{S}_1} \leq 18 \sum_{j=0}^{2} |c_j| (m_0^2 - m_j^2)^2 \frac{I_7}{(m_0^2+\omega^2)^2} \big\|\boldsymbol{A}\big\|_{L^1}. \tag{3.27}$$

The analysis of the operator $\mathcal{R}_{1,2}$ is more involved. Under conditions (2.7), we are not able to prove that $\mathcal{R}_{1,2}$ is trace-class. However we can compute first the $\mathbb{C}^4$–trace before taking the operator trace. We obtain

$$\mathrm{tr}_{\mathbb{C}^4} \mathcal{R}_{1,2} = 0, \tag{3.28}$$

since $\mathrm{tr}_{\mathbb{C}^4} \boldsymbol{\beta} = 0$.

Remark 3.2. By this argument, we do not prove that $\mathcal{R}_{1,2}$ is trace-class. Under the additional conditions

$$\sum_j c_j \, m_j = \sum_j c_j \, m_j^3 = 0,$$

the operator $\mathcal{R}_{1,2}$ becomes a trace-class operator, and its trace is equal to 0. This strategy however requires to introduce additional fictitious particles in our model. Introducing more fictitious particles in order to justify the computation of a term which is anyway 0 does not seem very reasonable from a physical point of view. This explains why we prefer here to first take the $\mathbb{C}^4$–trace.

As a consequence, we can conclude our estimate of the first order term by combining (3.27) and (3.28) in order to obtain

$$\begin{aligned}\int_{\mathbb{R}} \Big\| \mathrm{tr}_{\mathbb{C}^4} \big(R_1(\omega, \boldsymbol{A}) + R_1(-\omega, \boldsymbol{A})\big)\Big\|_{\mathfrak{S}_1} d\omega \\ \leq 36 \, I_7 \sum_{j=0}^{2} |c_j| \, \frac{(m_0^2 - m_j^2)^2}{m_0} \, \|\boldsymbol{A}\|_{L^1} \int_{\mathbb{R}} \frac{\omega^2 \, d\omega}{(1+\omega^2)^2}.\end{aligned} \tag{3.29}$$

The second and third order terms are treated following the same method, except that the algebra is a little more tedious. We start by writing that

$$\begin{aligned}R_n(\omega, \boldsymbol{A}) + R_n(-\omega, \boldsymbol{A}) = 2\omega^2 \sum_{j=0}^{2} c_j \sum_{k=0}^{n} \Big(\frac{1}{D_{m_j,0} - i\omega} \big(\boldsymbol{\alpha} \cdot A - V\big)\Big)^k \times \\ \times \frac{1}{D_{m_j,0}^2 + \omega^2} \Big(\big(\boldsymbol{\alpha} \cdot A - V\big) \frac{1}{D_{m_j,0} + i\omega}\Big)^{n-k}.\end{aligned}$$

We next expand as before using (3.19).

Estimate on the second order term. For the second order term, we are left with

$$\begin{aligned} R_2(\omega,\boldsymbol{A})+R_2(-\omega,\boldsymbol{A}) = -2\omega^2\sum_{j=0}^{2} c_j \times \\ \times\Big(\frac{\omega^2}{D_{m_j,0}^2+\omega^2}\Big((\boldsymbol{\alpha}\cdot A - V)\frac{1}{D_{m_j,0}^2+\omega^2}\Big)^2 - \sum_{k=0}^{2}\Big(\frac{D_{m_j,0}}{D_{m_j,0}^2+\omega^2}\times \\ \times\big(\boldsymbol{\alpha}\cdot A - V\big)\Big)^k \frac{1}{D_{m_j,0}^2+\omega^2}\Big((\boldsymbol{\alpha}\cdot A - V)\frac{D_{m_j,0}}{D_{m_j,0}^2+\omega^2}\Big)^{2-k}\Big), \end{aligned}$$

which may also be written as

$$\begin{aligned} R_2(\omega,\boldsymbol{A}) + R_2(-\omega,\boldsymbol{A}) = -2\omega^2\sum_{j=0}^{2} c_j\Big(\frac{1}{D_{m_j,0}^2+\omega^2}\big(\boldsymbol{\alpha}\cdot A - V\big)^2\frac{1}{D_{m_j,0}^2+\omega^2} \\ - \frac{1}{D_{m_j,0}^2+\omega^2}\Big(\big\{\boldsymbol{\alpha}\cdot A - V, D_{m_j,0}\big\}\frac{1}{D_{m_j,0}^2+\omega^2}\Big)^2\Big). \end{aligned} \tag{3.30}$$

Inserting

$$(\boldsymbol{\alpha}\cdot A - V)^2 = |A|^2 + V^2 - 2\,\boldsymbol{\alpha}\cdot A\,V,$$

and (3.22) into (3.30), we are led to

$$R_2(\omega,\boldsymbol{A}) + R_2(-\omega,\boldsymbol{A}) = -2\omega^2\big(\mathcal{R}_{2,1}+\mathcal{R}_{2,2}\big), \tag{3.31}$$

where

$$\begin{aligned} \mathcal{R}_{2,1} := \sum_{j=0}^{2} c_j\,\frac{1}{p^2+m_j^2+\omega^2}\Big(\Big(|A|^2+V^2-2\,\boldsymbol{\alpha}\cdot A\,V\Big)\frac{1}{p^2+m_j^2+\omega^2} \\ -4m_j^2\Big(V\,\frac{1}{p^2+m_j^2+\omega^2}\Big)^2 - \Big(\big(\big\{p, A - V\boldsymbol{\alpha}\big\}_{\mathbb{R}^3} + B\cdot\boldsymbol{\Sigma}\big)\frac{1}{p^2+m_j^2+\omega^2}\Big)^2\Big), \end{aligned}$$

and

$$\begin{aligned} \mathcal{R}_{2,2} := 2\sum_{j=0}^{2} c_j\,m_j\,\frac{1}{p^2+m_j^2+\omega^2}\times \\ \times\Big\{V\boldsymbol{\beta}\,\frac{1}{p^2+m_j^2+\omega^2}, \Big(\big\{p, A - V\boldsymbol{\alpha}\big\}_{\mathbb{R}^3} + B\cdot\boldsymbol{\Sigma}\Big)\frac{1}{p^2+m_j^2+\omega^2}\Big\}. \end{aligned}$$

The proof that $\mathcal{R}_{2,1}$ is trace-class is similar to the first order case, using (3.26). The final estimate is

$$\begin{aligned} \big\|\mathcal{R}_{2,1}\big\|_{\mathfrak{S}_1} \leq \sum_{j=0}^{2}|c_j|\Big(8\,I_7\frac{m_j^2-m_0^2}{(m_0^2+\omega^2)^2}\big\|\boldsymbol{A}\big\|_{L^2}\big\|B\big\|_{L^2} + I_8\frac{m_j^2-m_0^2}{(m_0^2+\omega^2)^{\frac{5}{2}}}\times \\ \times\Big(4m_j^2\big\|V\big\|_{L^2}^2 + \big\|B\big\|_{L^2}^2 + 8(m_j^2-m_0^2)\big\|\boldsymbol{A}\big\|_{L^2}^2\Big)\Big). \end{aligned}$$

Since

$$\mathrm{tr}_{\mathbb{C}^4}\,\mathcal{R}_{2,2} = 0, \tag{3.32}$$

as for the first-order term, our final estimate is

$$\int_{\mathbb{R}} \Big\| \operatorname{tr}_{\mathbb{C}^4} \big(R_2(\omega, A) + R_2(-\omega, A)\big) \Big\|_{\mathfrak{S}_1} d\omega$$
$$\leq \sum_{j=0}^{2} |c_j| \bigg(8\, I_7\, \frac{m_j^2 - m_0^2}{m_0} \big\|\boldsymbol{A}\big\|_{L^2} \big\|B\big\|_{L^2} \int_{\mathbb{R}} \frac{\omega^2\, d\omega}{(1+\omega^2)^2} + I_8\, \frac{m_j^2 - m_0^2}{m_0^2} \times$$
$$\times \Big(4m_j^2 \big\|V\big\|_{L^2}^2 + \big\|B\big\|_{L^2}^2 + 8(m_j^2 - m_0^2) \big\|\boldsymbol{A}\big\|_{L^2}^2 \Big) \int_{\mathbb{R}} \frac{\omega^2\, d\omega}{(1+\omega^2)^{\frac{5}{2}}} \bigg). \quad (3.33)$$

Estimate on the third order term. Similar computations give for the third order term

$$R_3(\omega, \boldsymbol{A}) + R_3(-\omega, \boldsymbol{A}) = \sum_{j=0}^{2} c_j \bigg(\frac{2\omega^2}{p^2 + m_j^2 + \omega^2} \Big(\big(\{p, A - V\boldsymbol{\alpha}\}_{\mathbb{R}^3} + B \cdot \boldsymbol{\Sigma}$$
$$- 2m_j V \boldsymbol{\beta} \big) \frac{1}{p^2 + m_j^2 + \omega^2} \Big)^3 - \frac{2\omega^2}{p^2 + m_j^2 + \omega^2} \bigg\{ \big(|A|^2 + V^2 - 2\,\boldsymbol{\alpha} \cdot A\, V \big)$$
$$\times \frac{1}{p^2 + m_j^2 + \omega^2}, \big(\{p, A - V\boldsymbol{\alpha}\}_{\mathbb{R}^3} + B \cdot \boldsymbol{\Sigma} - 2m_j V \boldsymbol{\beta} \big) \frac{1}{p^2 + m_j^2 + \omega^2} \bigg\} \bigg). \quad (3.34)$$

Using once again (3.26), we deduce

$$\int_{\mathbb{R}} \Big\| \operatorname{tr}_{\mathbb{C}^4} \big(R_3(\omega, \boldsymbol{A}) + R_3(-\omega, \boldsymbol{A})\big) \Big\|_{\mathfrak{S}_1} d\omega \leq K \sum_{j=0}^{2} |c_j| \int_{\mathbb{R}} \frac{\omega^2\, d\omega}{(1+\omega^2)^{\frac{13}{8}}} \times$$
$$\times \bigg(m_j I_8 \|V\|_{L^3}^3 + I_8 \|V\|_{L^4}^2 \|B\|_{L^2} + \frac{I_6 (I_8)^{\frac{1}{4}}}{m_j^{\frac{1}{4}}} \|B\|_{L^2}^2 \|V\|_{L^4} + \frac{(I_{16/3})^{\frac{3}{2}}}{m_j^{\frac{1}{2}}} \|B\|_{L^2}^3$$
$$+ m_j I_7 \|\boldsymbol{A}\|_{L^3} \|V\|_{L^3}^2 + \frac{(I_4)^{\frac{1}{4}} I_6}{m_j^{\frac{1}{4}}} \|B\|_{L^2}^2 \|\boldsymbol{A}\|_{L^4} + \frac{I_8}{m_j} \|\boldsymbol{A}\|_{L^3}^2 \|V\|_{L^3}$$
$$+ (m_j^2 - m_0^2) \Big(\frac{I_8}{m_j^2} \|\boldsymbol{A}\|_{L^4}^2 \|B\|_{L^2} + \frac{I_7}{m_j} \|\boldsymbol{A}\|_{L^3}^3 \Big) \bigg),$$

for some universal constant K.

Combining with (3.14), (3.15), (3.18), (3.29) and (3.33), we obtain (3.10), provided that $\boldsymbol{A}$ is in $L^1(\mathbb{R}^3, \mathbb{R}^3) \cap H^1(\mathbb{R}^3, \mathbb{R}^3)$. This concludes the proof of Proposition 3.1. □

4. Estimates involving the field energy

In Proposition 3.1 above we have shown that the operator

$$\operatorname{tr}_{\mathbb{C}^4} T_{\boldsymbol{A}} := \frac{1}{2} \sum_{j=0}^{2} c_j \operatorname{tr}_{\mathbb{C}^4} \big(|D_{m_j,0}| - |D_{m_j,\boldsymbol{A}}| \big),$$

is trace-class when $\boldsymbol{A}$ decays fast enough. More precisely, in the proof of Proposition 3.1, we have written

$$\begin{aligned} T_{\boldsymbol{A}} = \sum_{n=1}^{5} T_n(\boldsymbol{A}) + T_6'(\boldsymbol{A}) :=& \frac{1}{4\pi} \sum_{n=1}^{5} \int_{\mathbb{R}} \big(R_n(\omega, \boldsymbol{A}) + R_n(-\omega, \boldsymbol{A}) \big)\, d\omega \\ &+ \frac{1}{4\pi} \int_{\mathbb{R}} \big(R_6'(\omega, \boldsymbol{A}) + R_6'(-\omega, \boldsymbol{A}) \big)\, d\omega, \end{aligned} \tag{4.1}$$

with R_n and R_6' given by (3.8) and (3.9), and we have proved that the operators $\mathrm{tr}_{\mathbb{C}^4} T_n(\boldsymbol{A})$ and $\mathrm{tr}_{\mathbb{C}^4} T_6'(\boldsymbol{A})$ are trace-class. However our estimates involve non gauge-invariant quantities (some L^p norms of $\boldsymbol{A}$) and they require that $\boldsymbol{A}$ decays fast enough at infinity.

In this section, we establish better bounds on these different terms. We are interested in having estimates which only involve the field $\boldsymbol{F} = (-\nabla V, \operatorname{curl} A)$ through the norms $\|\nabla V\|_{L^2}$ and $\|\operatorname{curl} A\|_{L^2}$. Our simple estimate (3.14) on the sixth order only depends on the field $\boldsymbol{F}$. But we will also need to know that the sixth order is continuous, which will require some more work. For the other terms, we have to get the exact cancellations.

With these estimates at hand, it will be easy to show that $\mathcal{F}_{\mathrm{PV}}$ can be uniquely extended to a continuous function on the Coulomb-gauge homogeneous Sobolev space $\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$, as stated in Theorem 2.1, and which we do in the next section.

Remark 4.1. In the estimates of the previous section, it was not important that $\operatorname{div} A = 0$. We have to use this property now.

4.1. **The odd orders vanish.** The following lemma says that the trace of the odd order operators $\mathrm{tr}_{\mathbb{C}^4} T_1(\boldsymbol{A})$, $\mathrm{tr}_{\mathbb{C}^4} T_3(\boldsymbol{A})$ and $\mathrm{tr}_{\mathbb{C}^4} T_5(\boldsymbol{A})$ vanish. This consequence of the charge-conjugation invariance is sometimes called Furry's theorem [13].

Lemma 4.1 (The odd orders vanish)**.** *For $\boldsymbol{A} \in \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3, \mathbb{R}^4)$ and $n = 1, 3, 5$, we have*

$$\mathrm{tr}\left(\mathrm{tr}_{\mathbb{C}^4} T_n(\boldsymbol{A}) \right) = \frac{1}{4\pi} \int_{\mathbb{R}} \mathrm{tr}\left(\mathrm{tr}_{\mathbb{C}^4} \left(R_n(\omega, \boldsymbol{A}) + R_n(-\omega, \boldsymbol{A}) \right) \right) d\omega = 0. \tag{4.2}$$

Proof. Let $\mathcal{C}\psi := i\beta\alpha_2\overline{\psi}$ be the (anti-unitary) charge-conjugation operator. Since $\mathcal{C}\, D_{m_j,0}\, \mathcal{C}^{-1} = -D_{m_j,0}$, we have

$$\mathcal{C} \left(D_{m_j,0} \pm i\omega \right)^{-1} \mathcal{C}^{-1} = -\left(D_{m_j,0} \pm i\omega \right)^{-1}.$$

Similarly, since A and V are real-valued, we can write

$$\mathcal{C}\, \boldsymbol{\alpha} \cdot A\, \mathcal{C}^{-1} = \boldsymbol{\alpha} \cdot A \quad \text{and} \quad \mathcal{C}\, V\, \mathcal{C}^{-1} = V,$$

so that

$$\mathcal{C}\, R_n(\pm\omega, \boldsymbol{A})\, \mathcal{C}^{-1} = (-1)^n R_n(\pm\omega, \boldsymbol{A}). \tag{4.3}$$

At this stage, we can compute

$$\mathrm{tr}_{\mathbb{C}^4} \left(\mathcal{C} T \mathcal{C}^{-1} \right) = \mathrm{tr}_{\mathbb{C}^4} \overline{T}, \tag{4.4}$$

for any operator T on $L^2(\mathbb{R}^3, \mathbb{C}^4)$. Here, $\overline{T}$ refers to the operator defined as

$$\overline{T}(f) := \overline{T(\overline{f})}.$$

When $\mathrm{tr}_{\mathbb{C}^4} T$ is trace-class, so is the operator $\mathrm{tr}_{\mathbb{C}^4} \overline{T}$, and its trace is equal to

$$\mathrm{tr}\left(\mathrm{tr}_{\mathbb{C}^4} \overline{T}\right) = \overline{\mathrm{tr}(\mathrm{tr}_{\mathbb{C}^4} T)}. \tag{4.5}$$

As a consequence, the operator $\mathrm{tr}_{\mathbb{C}^4}(\mathcal{C}T\mathcal{C}^{-1})$ is trace-class, as soon as T is trace-class, and its trace is the complex conjugate of the trace of T.

Finally, recall that we have established in the proof of Proposition 3.1 that the operators $\mathrm{tr}_{\mathbb{C}^4}(R_n(\omega, \boldsymbol{A}) + R_n(-\omega, \boldsymbol{A}))$ are trace-class for $n = 1, 3, 5$. Combining (4.3) with (4.4) and (4.5), we obtain

$$\mathrm{tr}\left(\mathrm{tr}_{\mathbb{C}^4}\left(R_n(\omega, \boldsymbol{A}) + R_n(-\omega, \boldsymbol{A})\right)\right) \\ = (-1)^n \overline{\mathrm{tr}\left(\mathrm{tr}_{\mathbb{C}^4}\left(R_n(\omega, \boldsymbol{A}) + R_n(-\omega, \boldsymbol{A})\right)\right)}.$$

We deduce that the quantity $\mathrm{tr}\left(\mathrm{tr}_{\mathbb{C}^4}(R_n(\omega, \boldsymbol{A}) + R_n(-\omega, \boldsymbol{A}))\right)$ is purely imaginary when n is odd, so that the trace of $\mathrm{tr}_{\mathbb{C}^4} T_n(\boldsymbol{A})$ is purely imaginary. Since the operator $\mathrm{tr}_{\mathbb{C}^4} T_n(\boldsymbol{A})$ is self-adjoint, its trace is necessarily equal to 0. This gives Formula (4.2). □

4.2. **The second order term.** We now compute exactly the second order term $T_2(\boldsymbol{A})$ appearing in the decomposition of $T_{\boldsymbol{A}}$, assuming that $\boldsymbol{A}$ belongs to $H^1(\mathbb{R}^3, \mathbb{R}^4)$ and $\operatorname{div} A = 0$. We will verify that it only depends on the electromagnetic fields $E := -\nabla V$ and $B := \operatorname{curl} A$.

Lemma 4.2 (Formula for the second order term)**.** *For $\boldsymbol{A} \in \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3) \cap L^2(\mathbb{R}^3, \mathbb{R}^4)$, we have*

$$\mathrm{tr}\left(\mathrm{tr}_{\mathbb{C}^4} T_2(\boldsymbol{A})\right) = \frac{1}{8\pi} \int_{\mathbb{R}^3} M(k)\left(|\widehat{B}(k)|^2 - |\widehat{E}(k)|^2\right) dk := \mathcal{F}_2(\boldsymbol{F}), \tag{4.6}$$

where M is the function defined in (2.16) *and $\boldsymbol{F} = (E, B)$.*

Proof. In the course of the proof of Proposition 3.1, we have shown that the operator $\mathrm{tr}_{\mathbb{C}^4} T_2(\boldsymbol{A})$ is trace-class when $\boldsymbol{A} \in H^1(\mathbb{R}^3, \mathbb{R}^3)$ (see inequality (3.33)). As a consequence, its trace is well-defined and given by

$$\mathrm{tr}\left(\mathrm{tr}_{\mathbb{C}^4} T_2(\boldsymbol{A})\right) = \int_{\mathbb{R}^3} \widehat{\left(\mathrm{tr}_{\mathbb{C}^4} T_2(\boldsymbol{A})\right)}(p, p)\, dp. \tag{4.7}$$

Here, $\widehat{\mathrm{tr}_{\mathbb{C}^4} T_2(\boldsymbol{A})}$ refers to the Fourier transform of the trace-class operator $\mathrm{tr}_{\mathbb{C}^4} T_2(\boldsymbol{A})$. Our convention for the Fourier transform of a trace-class operator T is the following

$$\widehat{T}(p, q) := \frac{1}{(2\pi)^3} \int_{\mathbb{R}^6} T(x, y) e^{-ip\cdot x} e^{iq\cdot y}\, dx\, dy.$$

In view of (3.31), the operator $\mathrm{tr}_{\mathbb{C}^4} T_2(\boldsymbol{A})$ is given by

$$\begin{aligned}\mathrm{tr}_{\mathbb{C}^4} T_2(\boldsymbol{A})(p,p) = \frac{2}{\pi}\int_{\mathbb{R}} \sum_{j=0}^{2} c_j \frac{1}{p^2+m_j^2+\omega^2}\bigg(&- \big(|A|^2+V^2\big)\frac{1}{p^2+m_j^2+\omega^2} \\ &+ \Big(\big\{p,A\big\}_{\mathbb{R}^3}\frac{1}{p^2+m_j^2+\omega^2}\Big)^2 + \sum_{k=1}^{3} B_k \frac{1}{p^2+m_j^2+\omega^2} B_k \frac{1}{p^2+m_j^2+\omega^2} \\ &+ \sum_{k=1}^{3} \big\{p_k,V\big\}\frac{1}{p^2+m_j^2+\omega^2}\big\{p_k,V\big\}\frac{1}{p^2+m_j^2+\omega^2} \\ &+ 4m_j^2\Big(V\frac{1}{p^2+m_j^2+\omega^2}\Big)^2\bigg)\omega^2\,d\omega.\end{aligned} \tag{4.8}$$

Since A is written in Coulomb gauge, we deduce that

$$\mathrm{tr}\,\big(\,\mathrm{tr}_{\mathbb{C}^4}\,T_2(\boldsymbol{A})\big) = \sum_{k=1}^{3} \mathcal{T}_{2,k}, \tag{4.9}$$

where

$$\mathcal{T}_{2,1} := -\frac{1}{\sqrt{2}\pi^{\frac{5}{2}}}\int_{\mathbb{R}^4}\sum_{j=0}^{2} c_j \frac{\omega^2\,d\omega\,dp}{(p^2+m_j^2+\omega^2)^2}\,\big(\widehat{|A|^2}(0)+\widehat{V^2}(0)\big), \tag{4.10}$$

$$\begin{aligned}\mathcal{T}_{2,2} &:= \frac{1}{\pi^4}\int_{\mathbb{R}^7}\sum_{j=0}^{2} c_j \frac{dk\,\omega^2\,d\omega\,dp}{(p^2+m_j^2+\omega^2)^2((p-k)^2+m_j^2+\omega^2)}\times \\ &\qquad\qquad \times\Big(\big(p\cdot\widehat{A}(k)\big)\big(p\cdot\widehat{A}(-k)\big)+\big(p^2+m_j^2\big)|\widehat{V}(k)|^2\Big) \\ &:= \mathcal{T}_{2,2}(A)+\mathcal{T}_{2,2}(V),\end{aligned} \tag{4.11}$$

and

$$\mathcal{T}_{2,3} := \frac{1}{4\pi^4}\int_{\mathbb{R}^7}\sum_{j=0}^{2} c_j \frac{k^2|\widehat{A}(k)|^2+(k^2-4p\cdot k)|\widehat{V}(k)|^2}{(p^2+m_j^2+\omega^2)^2((p-k)^2+m_j^2+\omega^2)}\,dk\,\omega^2\,d\omega\,dp. \tag{4.12}$$

We next use the following *Ward identities* [45]

$$\begin{aligned}&\int_{\mathbb{R}^3}\sum_{j=0}^{2} c_j \frac{p_m p_n\,dp}{(p^2+m_j^2+\omega^2)^2((p-k)^2+m_j^2+\omega^2)} \\ &\qquad = \int_{\mathbb{R}^3}\sum_{j=0}^{2} c_j \frac{(k_m-q_m)(k_n-q_n)\,dq}{((q-k)^2+m_j^2+\omega^2)^2(q^2+m_j^2+\omega^2)},\end{aligned} \tag{4.13}$$

for all $(m,n)\in\{1,2,3\}^2$ and all $k\in\mathbb{R}^3$. This equation is nothing else than a change of variables $p=k-q$, which makes perfect sense thanks to conditions (2.7) which guarantee the convergence of the integral. Its importance is well-known in the Physics literature, see, e.g., [30, Sec. 7.4].

Since $\operatorname{div} A = 0$, we infer that

$$\mathcal{T}_{2,2}(A) = -\frac{1}{4\pi^4}\int_{\mathbb{R}^4}\sum_{m=1}^{3}\sum_{n=1}^{3}\widehat{A_m}(k)\widehat{A_n}(-k)\,dk\,\omega^2\,d\omega\times$$
$$\times\int_{\mathbb{R}^3}\sum_{j=0}^{2}c_j p_m\partial_{p_n}\Big(\frac{1}{(p^2+m_j^2+\omega^2)((p-k)^2+m_j^2+\omega^2)}\Big)\,dp.$$

Integrating by parts, we are led to

$$\mathcal{T}_{2,2}(A) = \frac{1}{4\pi^4}\int_{\mathbb{R}^7}\sum_{j=0}^{2}c_j\frac{|\widehat{A}(k)|^2\,dk\,\omega^2\,d\omega\,dp}{(p^2+m_j^2+\omega^2)((p-k)^2+m_j^2+\omega^2)}. \tag{4.14}$$

Similarly, we can compute

$$\mathcal{T}_{2,2}(V) = \frac{1}{\pi^4}\int_{\mathbb{R}^7}\sum_{j=0}^{2}c_j\frac{|\widehat{V}(k)|^2\,dk\,\omega^2\,d\omega\,dp}{(p^2+m_j^2+\omega^2)((p-k)^2+m_j^2+\omega^2)}$$
$$-\frac{1}{\pi^4}\int_{\mathbb{R}^7}\sum_{j=0}^{2}c_j\frac{|\widehat{V}(k)|^2\,dk\,\omega^4\,d\omega\,dp}{(p^2+m_j^2+\omega^2)^2((p-k)^2+m_j^2+\omega^2)}.$$

Integrating by parts with respect to ω, one can check that

$$\int_{\mathbb{R}^4}\sum_{j=0}^{2}c_j\frac{\omega^4\,d\omega\,dp}{(p^2+m_j^2+\omega^2)^2((p-k)^2+m_j^2+\omega^2)}$$
$$=\frac{3}{4}\int_{\mathbb{R}^4}\sum_{j=0}^{2}c_j\frac{\omega^2\,d\omega\,dp}{(p^2+m_j^2+\omega^2)((p-k)^2+m_j^2+\omega^2)},$$

so that

$$\mathcal{T}_{2,2}(V) = \frac{1}{4\pi^4}\int_{\mathbb{R}^7}\sum_{j=0}^{2}c_j\frac{|\widehat{V}(k)|^2\,dk\,\omega^2\,d\omega\,dp}{(p^2+m_j^2+\omega^2)((p-k)^2+m_j^2+\omega^2)}. \tag{4.15}$$

On the other hand, since A and V are real-valued, we have

$$\widehat{|A|^2}(0)+\widehat{V^2}(0) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int_{\mathbb{R}^3}\big(|\widehat{A}(k)|^2+|\widehat{V}(k)|^2\big)\,dk,$$

hence

$$\mathcal{T}_{2,1} = -\frac{1}{4\pi^4}\int_{\mathbb{R}^7}\sum_{j=0}^{2}c_j\frac{|\widehat{A}(k)|^2+|\widehat{V}(k)|^2}{(p^2+m_j^2+\omega^2)^2}\,\omega^2\,d\omega\,dk\,dp.$$

Combining with (4.14) and (4.15), we arrive at

$$\mathcal{T}_{2,1}+\mathcal{T}_{2,2} = \frac{1}{4\pi^4}\int_{\mathbb{R}^7}\sum_{j=0}^{2}c_j\frac{\big(2p\cdot k-|k|^2\big)\big(|\widehat{A}(k)|^2+|\widehat{V}(k)|^2\big)}{(p^2+m_j^2+\omega^2)^2((p-k)^2+m_j^2+\omega^2)}\,\omega^2\,d\omega\,dk\,dp.$$

In view of (4.9) and (4.12), this provides

$$\operatorname{tr}\big(\operatorname{tr}_{\mathbb{C}^4}T_2(A)\big) = \int_{\mathbb{R}^3}G(k)\big(|\widehat{A}(k)|^2-|\widehat{V}(k)|^2\big)\,dk, \tag{4.16}$$

where

$$G(k) := \frac{1}{2\pi^4} \int_{\mathbb{R}^4} \sum_{j=0}^{2} c_j \frac{p \cdot k \, \omega^2 \, d\omega \, dp}{(p^2 + m_j^2 + \omega^2)^2((p-k)^2 + m_j^2 + \omega^2)}.$$

We next use the identity

$$\frac{1}{a^2 b} = \int_0^1 \left(\int_0^\infty s^2 e^{-s(ua+(1-u)b)} \, ds \right) u \, du,$$

see [16, Chap. 5], to rewrite

$$\begin{aligned} G(k) = \frac{1}{2\pi^4} \int_{\mathbb{R}^4} \sum_{j=0}^{2} c_j \, \omega^2 \, d\omega \, p \cdot k \, dp \times \\ \times \left(\int_0^1 \int_0^\infty e^{-s(p^2+m_j^2+\omega^2)-s(1-u)(k^2-2p\cdot k)} \, s^2 \, ds \, u \, du \right). \end{aligned} \tag{4.17}$$

Using conditions (2.7), we can invoke Fubini's theorem to recombine the integrals in (4.17) as

$$\begin{aligned} G(k) = \frac{1}{2\pi^4} \int_0^1 \int_0^\infty \sum_{j=0}^{2} c_j \, e^{-s(m_j^2+(1-u)k^2)} s^2 \, ds \, u \, du \times \\ \times \int_{\mathbb{R}^3} p \cdot k \, e^{-s(p^2-2(1-u)p\cdot k)} \left(\int_{\mathbb{R}} e^{-s\omega^2} \omega^2 \, d\omega \right) dp. \end{aligned}$$

Since

$$\int_{\mathbb{R}} e^{-s\omega^2} \omega^2 \, d\omega = \frac{\sqrt{\pi}}{2s^{\frac{3}{2}}},$$

and

$$\begin{aligned} \int_{\mathbb{R}^3} p \cdot k \, e^{-s(p^2-2(1-u)p\cdot k)} \, dp &= k \cdot \nabla \left(\int_{\mathbb{R}^3} e^{p\cdot x - sp^2 - 2s(1-u)p\cdot k} \, dp \right)_{|x=0} \\ &= \left(\frac{\pi}{s} \right)^{\frac{3}{2}} (1-u) k^2 e^{s(1-u)^2 k^2}, \end{aligned}$$

we deduce that

$$G(k) = \frac{k^2}{4\pi^2} \int_0^1 \int_0^\infty \sum_{j=0}^{2} c_j \, e^{-s(m_j^2+u(1-u)k^2)} s^{-1} \, ds \, u(1-u) \, du. \tag{4.18}$$

Integrating by parts, we now compute

$$\begin{aligned} \int_0^\infty \sum_{j=0}^{2} c_j \, e^{-s(m_j^2+u(1-u)k^2)} s^{-1} \, ds \\ = \int_0^\infty \sum_{j=0}^{2} c_j \, \log(s) e^{-s(m_j^2+u(1-u)k^2)} \, (m_j^2 + u(1-u)k^2) \, ds, \end{aligned}$$

which is justified again thanks to conditions (2.7). Letting $\sigma = s(m_j^2+u(1-u)k^2)$, we infer again from (2.7) that

$$\int_0^\infty \sum_{j=0}^{2} c_j e^{-s(m_j^2+u(1-u)k^2)} s^{-1}\, ds = \int_0^\infty \sum_{j=0}^{2} c_j \log\Big(\frac{\sigma}{m_j^2+u(1-u)k^2}\Big) e^{-\sigma}\, d\sigma$$
$$= -\sum_{j=0}^{2} c_j\, \log(m_j^2+u(1-u)k^2).$$

Inserting into (4.18), we get

$$G(k) = -\frac{k^2}{4\pi^2}\int_0^1 \sum_{j=0}^{2} c_j\, u(1-u)\, \log(m_j^2+u(1-u)k^2)\, du = \frac{k^2}{8\pi} M(k).$$

Combining with (4.16), we obtain Formula (4.6). □

We complete our analysis of the second order term by giving the main properties of the function M.

Lemma 4.3 (Main properties of M)**.** *Assume that c_j and m_j satisfy* (2.10)*. The function M given by* (2.16) *is well-defined and positive on $\mathbb{R}^3$, and satisfies*

$$0 < M(k) \le M(0) = \frac{2\,\log(\Lambda)}{3\pi},$$

where Λ is defined by (2.9)*. Moreover,*

$$\frac{2\,\log(\Lambda)}{3\pi} - M(k) \to \frac{|k|^2}{4\pi}\int_0^1 \frac{z^2-z^4/3}{1+|k|^2(1-z^2)/4}\, dz,$$

when $m_1 \to \infty$ and $m_2 \to \infty$.

Proof. In view of (2.16), the function M is well-defined on $\mathbb{R}^3$. Concerning its positivity, we set

$$\Phi(t) := \sum_{j=0}^{2} c_j\, \log(m_j^2+t),$$

for all $t \ge 0$. Using (2.8), we compute

$$\Phi'(t) = \sum_{j=0}^{2} \frac{c_j}{m_j^2+t} = \frac{(m_1^2-m_0^2)(m_2^2-m_0^2)}{(m_0^2+t)(m_1^2+t)(m_2^2+t)} > 0.$$

Since $\Phi(0) = -2\log\Lambda < 0$ and

$$\Phi(t) = \sum_{j=0}^{2} c_j\, \log\Big(1+\frac{m_j^2}{t}\Big) \to 0, \text{ as } t \to \infty,$$

by (2.7), we deduce that

$$-2\log\Lambda < \Phi(t) < 0,$$

for all $t > 0$. Inserting into (2.16), we obtain (2.17).

As for (2.18), we first write

$$\begin{aligned} M(k) =& -\frac{2}{\pi}\int_0^1 \sum_{j=0}^{2} c_j\, u(1-u)\left(\log(m_j^2)+\log\left(1+\frac{u(1-u)k^2}{m_j^2}\right)\right) du \\ =& \frac{2\,\log\Lambda}{3\pi} - \frac{2}{\pi}\int_0^1 \sum_{j=0}^{2} c_j\, u(1-u)\,\log\left(1+\frac{u(1-u)k^2}{m_j^2}\right) du. \end{aligned}$$

When $m_1 \to \infty$ and $m_2 \to \infty$, we infer that

$$\frac{2\,\log\Lambda}{3\pi} - M(k) \to \frac{2}{\pi}\int_0^1 u(1-u)\,\log\left(1+u(1-u)k^2\right) du.$$

Integrating by parts, we compute

$$\int_0^1 u(1-u)\,\log\left(1+u(1-u)k^2\right) du = -\int_0^1 \frac{(\frac{u^2}{2}-\frac{u^3}{3})(1-2u)\,du}{1+u(1-u)k^2},$$

so that it only remains to set $z = 1-2u$ to derive (2.18). This concludes the proof of Lemma 4.3. □

4.3. **The fourth order term.** Our goal is now to provide an estimate on the fourth order term $T_4(\boldsymbol{A})$. We have estimated this term in (3.18), and we know that $T_4(\boldsymbol{A})$ is trace-class when $\boldsymbol{A} \in L^4(\mathbb{R}^3,\mathbb{R}^4)$. Here, we want to get an estimate involving only the norm of $\boldsymbol{A}$ in $\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$.

Lemma 4.4 (Estimate for the fourth order term)**.** *Let $\boldsymbol{A} = (A,V) \in L^4(\mathbb{R}^3,\mathbb{R}^4) \cap \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$ and set $B := \operatorname{curl} A$ and $E := -\nabla V$. There exists a universal constant K such that*

$$\left|\operatorname{tr}\left(\operatorname{tr}_{\mathbb{C}^4} T_4(\boldsymbol{A})\right)\right| = \left|\operatorname{tr} T_4(\boldsymbol{A})\right| \leq K\left(\sum_{j=0}^{2}\frac{|c_j|}{m_j}\right)\left(\|B\|_{L^2}+\|E\|_{L^2}\right)^4. \quad (4.19)$$

Proof. Arguing as in the proof of Proposition 3.1 (see the proof of Formulas (3.31) and (3.34)), we decompose $T_4(\boldsymbol{A})$ as

$$T_4(\boldsymbol{A}) = T_{4,1}(\boldsymbol{A}) - T_{4,2}(\boldsymbol{A}) + T_{4,3}(\boldsymbol{A}), \quad (4.20)$$

where

$$T_{4,1}(\boldsymbol{A}) := \frac{1}{2\pi}\int_{\mathbb{R}}\sum_{j=0}^{2} c_j\,\omega^2\,d\omega\,\frac{1}{p^2+m_j^2+\omega^2}\left(\mathcal{W}_2\,\frac{1}{p^2+m_j^2+\omega^2}\right)^2, \quad (4.21)$$

$$\begin{aligned} T_{4,2}(\boldsymbol{A}) :=& \frac{1}{2\pi}\int_{\mathbb{R}}\sum_{j=0}^{2} c_j\,\omega^2\,d\omega\,\frac{1}{p^2+m_j^2+\omega^2}\left(\mathcal{W}_2\,\frac{1}{p^2+m_j^2+\omega^2}\times\right. \\ &\times\left(\mathcal{W}_1\,\frac{1}{p^2+m_j^2+\omega^2}\right)^2 + \left(\mathcal{W}_1\,\frac{1}{p^2+m_j^2+\omega^2}\right)^2\mathcal{W}_2\,\frac{1}{p^2+m_j^2+\omega^2} \\ &\left.+\,\mathcal{W}_1\,\frac{1}{p^2+m_j^2+\omega^2}\,\mathcal{W}_2\,\frac{1}{p^2+m_j^2+\omega^2}\,\mathcal{W}_1\,\frac{1}{p^2+m_j^2+\omega^2}\right), \end{aligned} \quad (4.22)$$

and

$$T_{4,3}(\boldsymbol{A}) := \frac{1}{2\pi}\int_{\mathbb{R}}\sum_{j=0}^{2} c_j\,\omega^2\,d\omega\,\frac{1}{p^2+m_j^2+\omega^2}\left(\mathcal{W}_1\,\frac{1}{p^2+m_j^2+\omega^2}\right)^4. \quad (4.23)$$

Here, we have set for shortness,

$$\mathcal{W}_1 := \big\{p, A - V\boldsymbol{\alpha}\big\}_{\mathbb{R}^3} + B\cdot\boldsymbol{\Sigma} - 2m_jV\boldsymbol{\beta},$$

and

$$\mathcal{W}_2 := |A|^2 + V^2 - 2\big(\boldsymbol{\alpha}\cdot A\big)V.$$

Let us now explain our method to establish (4.19). When looking at $\mathcal{T}_{4,k}$ with $k = 1, 2, 3$, we are worried about several terms. First the function $\mathcal{W}_2$ does not decay too fast, it is only in $L^3(\mathbb{R}^3)$ if we only want to use the L^6 norm of $\boldsymbol{A}$. Furthermore, it involves quantities which are not gauge invariant. Similarly, the term involving p in $\mathcal{W}_1$ is clearly the worst. It also involves non-gauge invariant quantities. On the other hand, the term involving B is in $L^2(\mathbb{R}^3)$ and it is gauge invariant. The term involving V alone is also not gauge invariant but it has the matrix $\boldsymbol{\beta}$ which will help us, and it has no p. Since the result should be gauge invariant, these terms cannot be a problem. They should not contribute to the total (fourth order) energy.

In order to see this, we use the following technique. In Formulas (4.21)–(4.23), we commute all the operators involving p in order to place them either completely on the left or completely on the right. We have to commute the terms $(p^2+m_j^2+\omega^2)^{-1}$ as well as the p appearing in $\mathcal{W}_1$. We think that it does not matter how many terms we put on the left and on the right. It is just important to have some functions of p on both sides (to get a trace-class operator under suitable assumptions on $\boldsymbol{A}$), and we do not want to put them all on one side only. All the commutators obtained by these manipulations are better behaved and they will be estimated using the Kato-Seiler-Simon inequality (2.5), only in terms of $\|\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}$.

In the end of the process, we will be left with a sum of terms of the form

$$\frac{|p|^c}{(p^2+m_j^2+\omega^2)^a}\,f(x)\,\frac{|p|^d}{(p^2+m_j^2+\omega^2)^b},$$

where $f(x)$ is $\mathcal{W}_2^2$ or a product of $\mathcal{W}_2$ with some of the functions appearing in $\mathcal{W}_1$, or only these functions. For instance, when we take the trace, the worst term involving only V is

$$\left(\int_{\mathbb{R}^3} V^4\right)\left(\int_{\mathbb{R}^3}\frac{dp}{(p^2+m_j^2+\omega^2)^3} + 3\int_{\mathbb{R}^3}\frac{|p|^2\,dp}{(p^2+m_j^2+\omega^2)^4} + \int_{\mathbb{R}^3}\frac{|p|^4\,dp}{(p^2+m_j^2+\omega^2)^5}\right).$$

Here the integrals over p come respectively from $\mathcal{T}_{4,1}$, $\mathcal{T}_{4,2}$ and $\mathcal{T}_{4,3}$ and they behave exactly like $(\omega^2+m_j^2)^{-5/2}$. So we run into problems when we want to multiply by ω^2 and then integrate with respect to ω. But this term cannot be a problem here because $\int_{\mathbb{R}^3} V^4$ is not a gauge invariant quantity. This is where the Pauli-Villars scheme helps us. Not only these integrals

will become well-defined, but also their sum will simply vanish because the regularization was precisely designed to preserve gauge invariance.

But before we explain all this in details, let us indicate how to handle the multiple commutators that we get when commuting the operators involving p. We start with $T_{4,1}$, for instance. Following the general strategy explained above, we write

$$T_{4,1}(\boldsymbol{A}) = \frac{1}{2\pi}\int_{\mathbb{R}}\sum_{j=0}^{2} c_j\,\omega^2\,d\omega\bigg(\frac{1}{p^2+m_j^2+\omega^2}\,(\mathcal{W}_2)^2\frac{1}{(p^2+m_j^2+\omega^2)^2} + \frac{1}{p^2+m_j^2+\omega^2}\,\mathcal{W}_2\Big[\frac{1}{(p^2+m_j^2+\omega^2)},\mathcal{W}_2\Big]\frac{1}{p^2+m_j^2+\omega^2}\bigg),$$

where, as usual, $[S,T] := ST - TS$. We notice that

$$\Big[\mathcal{W}_2, \frac{1}{p^2+m_j^2+\omega^2}\Big] = \frac{1}{p^2+m_j^2+\omega^2}\,\big[p^2,\mathcal{W}_2\big]\,\frac{1}{p^2+m_j^2+\omega^2},$$

while

$$\big[p^2,\mathcal{W}_2\big] = p\big[p,\mathcal{W}_2\big] + \big[p,\mathcal{W}_2\big]p = -i\big\{p,\nabla\mathcal{W}_2\big\}_{\mathbb{R}^3}.$$

Hence, we have

$$T_{4,1}(\boldsymbol{A}) = \frac{1}{2\pi}\int_{\mathbb{R}}\sum_{j=0}^{2} c_j\,\omega^2\,d\omega\bigg(\frac{1}{p^2+m_j^2+\omega^2}\,(\mathcal{W}_2)^2\frac{1}{(p^2+m_j^2+\omega^2)^2} + i\frac{1}{p^2+m_j^2+\omega^2}\,\mathcal{W}_2\,\frac{1}{p^2+m_j^2+\omega^2}\,\big\{p,\nabla\mathcal{W}_2\big\}_{\mathbb{R}^3}\,\frac{1}{(p^2+m_j^2+\omega^2)^2}\bigg), \quad (4.24)$$

where

$$\nabla\mathcal{W}_2 = 2A\cdot\nabla A + 2V\,\nabla V - 2V\,\big(\boldsymbol{\alpha}\cdot\nabla A\big) - 2\nabla V\,\big(\boldsymbol{\alpha}\cdot A\big).$$

We then argue as in the proof of Proposition 3.1. We use that $\mathcal{W}_2 \in L^3(\mathbb{R}^3)$, with

$$\|\mathcal{W}_2\|_{L^3} \le K\|\boldsymbol{A}\|_{L^6}^2 \le K\|\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}^2,$$

and that $\nabla\mathcal{W}_2 \in L^{\frac{3}{2}}(\mathbb{R}^3)$, with

$$\|\nabla\mathcal{W}_2\|_{L^{\frac{3}{2}}} \le K\|\boldsymbol{A}\|_{L^6}\|\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \le K\|\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}^2,$$

by the Sobolev inequality. By the Kato-Seiler-Simon inequality (2.5), we obtain for the term involving $p\cdot\nabla\mathcal{W}_2$,

$$\begin{aligned}
&\Big\|\frac{1}{p^2+m_j^2+\omega^2}\,\mathcal{W}_2\,\frac{1}{p^2+m_j^2+\omega^2}\,p\cdot\nabla\mathcal{W}_2\,\frac{1}{(p^2+m_j^2+\omega^2)^2}\Big\|_{\mathfrak{S}_1}\\
&\quad\le K\Big\|\frac{1}{p^2+m_j^2+\omega^2}\,\mathcal{W}_2\Big\|_{\mathfrak{S}_3}\Big\|\frac{|p|}{p^2+m_j^2+\omega^2}|\nabla\mathcal{W}_2|^{\frac{1}{4}}\Big\|_{\mathfrak{S}_6}\times\\
&\qquad\times\Big\||\nabla\mathcal{W}_2|^{\frac{3}{4}}\frac{1}{(p^2+m_j^2+\omega^2)^2}\Big\|_{\mathfrak{S}_2}\\
&\quad\le \frac{K}{(m_j^2+\omega^2)^2}\big\|\boldsymbol{A}\big\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}^4,
\end{aligned}$$

for some universal constant K. The argument is exactly the same for the term involving $\nabla\mathcal{W}_2 \cdot p$ instead of $p \cdot \nabla\mathcal{W}_2$. Therefore, we obtain the bound

$$\int_{\mathbb{R}} \sum_{j=0}^{2} |c_j| \left\| \frac{1}{(p^2+m_j^2+\omega^2)^3} \left\{ p, \nabla\mathcal{W}_2 \right\}_{\mathbb{R}^3} \frac{1}{p^2+m_j^2+\omega^2} \mathcal{W}_2 \right\|_{\mathfrak{S}_1} \omega^2 \, d\omega \\ \leq K \left(\sum_{j=0}^{2} \frac{|c_j|}{m_j} \right) \|\boldsymbol{A}\|^4_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}.$$

In particular, we have shown that the operator $T_{4,1}(\boldsymbol{A})$ can be written in the form

$$T_{4,1}(\boldsymbol{A}) = \mathcal{T}_{4,1}(\boldsymbol{A}) + \mathcal{S}_{4,1}(\boldsymbol{A}), \tag{4.25}$$

with

$$\left\| \mathcal{T}_{4,1}(\boldsymbol{A}) \right\|_{\mathfrak{S}_1} \leq K \left(\sum_{j=0}^{2} \frac{|c_j|}{m_j} \right) \|\boldsymbol{A}\|^4_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}, \tag{4.26}$$

and

$$\mathcal{S}_{4,1}(\boldsymbol{A}) := \frac{1}{2\pi} \int_{\mathbb{R}} \sum_{j=0}^{2} c_j \, \frac{1}{p^2+m_j^2+\omega^2} \left(\mathcal{W}_2 \right)^2 \frac{1}{(p^2+m_j^2+\omega^2)^2} \, \omega^2 \, d\omega. \tag{4.27}$$

By the Kato-Seiler-Simon inequality, this term is trace-class when $\boldsymbol{A} \in L^4(\mathbb{R}^3, \mathbb{R}^4)$ and conditions (2.7) are fulfilled. On the other hand, there is no evidence that the trace-class norm of $\mathcal{S}_{4,1}(\boldsymbol{A})$ can be bounded using only the norm $\|\nabla \boldsymbol{A}\|_{L^2}$. Fortunately, this term will cancel with the other ones of the same type, as we will explain later.

Our strategy to handle the operators $T_{4,2}(\boldsymbol{A})$ and $T_{4,3}(\boldsymbol{A})$ follows exactly the same lines. We first simplify the expressions of $T_{4,2}(\boldsymbol{A})$ and $T_{4,3}(\boldsymbol{A})$ by discarding the terms containing the operator $B \cdot \boldsymbol{\Sigma}$. Concerning $T_{4,3}(\boldsymbol{A})$, we can compute

$$\left\| \frac{1}{p^2+m_j^2+\omega^2} \Big(\mathcal{W}_1 \, \frac{1}{p^2+m_j^2+\omega^2} \Big)^3 B \cdot \boldsymbol{\Sigma} \, \frac{1}{p^2+m_j^2+\omega^2} \right\|_{\mathfrak{S}_1} \\ \leq \frac{K}{(m_j^2+\omega^2)^2} \, \|B\|_{L^2} \Big(\|\nabla \boldsymbol{A}\|^3_{L^2} + \frac{m_j^3}{(m_j^2+\omega^2)^{\frac{3}{2}}} \|\nabla V\|^3_{L^2} + \|B\|^3_{L^2} \Big),$$

so that

$$T_{4,3}(\boldsymbol{A}) = \mathcal{T}^a_{4,3}(\boldsymbol{A}) + \frac{1}{2\pi} \int_{\mathbb{R}} \sum_{j=0}^{2} \frac{c_j \, \omega^2 \, d\omega}{p^2+m_j^2+\omega^2} \left(\big(\mathcal{W}_1 - B \cdot \boldsymbol{\Sigma} \big) \, \frac{1}{p^2+m_j^2+\omega^2} \right)^4,$$

with

$$\left\| \mathcal{T}^a_{4,3}(\boldsymbol{A}) \right\|_{\mathfrak{S}_1} \leq K \left(\sum_{j=0}^{2} \frac{|c_j|}{m_j} \right) \|\boldsymbol{A}\|^4_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}. \tag{4.28}$$

We next commute, as above, the operator $\mathcal{W}_1 - B \cdot \mathbf{\Sigma}$ with the operator $1/(p^2 + m_j^2 + \omega^2)$ in order to establish that

$$\begin{aligned}
&\frac{1}{2\pi} \int_{\mathbb{R}} \omega^2 \, d\omega \sum_{j=0}^{2} c_j \frac{1}{p^2 + m_j^2 + \omega^2} \bigg(\left(\mathcal{W}_1 - B \cdot \mathbf{\Sigma} \right) \frac{1}{p^2 + m_j^2 + \omega^2} \bigg)^4 \\
&= \mathcal{T}_{4,3}^b(\boldsymbol{A}) + \frac{1}{2\pi} \int_{\mathbb{R}} \omega^2 \, d\omega \sum_{j=0}^{2} c_j \times \\
&\times \frac{1}{(p^2 + m_j^2 + \omega^2)^4} \Big(\big\{ p, A - V\boldsymbol{\alpha} \big\}_{\mathbb{R}^3} - 2 m_j V \boldsymbol{\beta} \Big)^4 \frac{1}{p^2 + m_j^2 + \omega^2},
\end{aligned}$$

where $\mathcal{T}_{4,3}^b(\boldsymbol{A})$ also satisfies (4.28). Finally, we use that

$$\big\{ p, A - \boldsymbol{\alpha} \cdot V \big\}_{\mathbb{R}^3} = 2p \cdot \big(A - \boldsymbol{\alpha} \cdot V \big) - i \boldsymbol{\alpha} \cdot \nabla V,$$

as well as the anti-commutation formulas for the matrices $\boldsymbol{\alpha}_k$ and $\boldsymbol{\beta}$, to obtain the formula

$$\begin{aligned}
&\frac{1}{2\pi} \int_{\mathbb{R}} \omega^2 \, d\omega \sum_{j=0}^{2} c_j \frac{1}{(p^2 + m_j^2 + \omega^2)^4} \times \\
&\qquad \times \Big(\big\{ p, A - V\boldsymbol{\alpha} \big\}_{\mathbb{R}^3} - 2 m_j V \boldsymbol{\beta} \Big)^4 \frac{1}{p^2 + m_j^2 + \omega^2} = \mathcal{T}_{4,3}^c(\boldsymbol{A}) + \mathcal{S}_{4,3}(\boldsymbol{A}),
\end{aligned}$$

with $\mathcal{T}_{4,3}^c(\boldsymbol{A})$ satisfying again (4.28), and

$$\begin{aligned}
\mathcal{S}_{4,3}(\boldsymbol{A}) := \frac{8}{\pi} \int_{\mathbb{R}} \omega^2 \, d\omega \sum_{j=0}^{2} c_j \, \frac{1}{(p^2 + m_j^2 + \omega^2)^4} \bigg(& (p^2 + m_j^2)^2 V^4 \\
& - 4(p^2 + m_j^2)(m_j \boldsymbol{\beta} + p \cdot \boldsymbol{\alpha})(p \cdot A) V^3 \boldsymbol{\beta} + 6(p^2 + m_j^2) \sum_{l=1}^{3} p_l (p \cdot A) A_\ell V^2 \\
& - 4 m_j \sum_{l=1}^{3} \sum_{m=1}^{3} p_l p_m (m_j \boldsymbol{\beta} + p \cdot \boldsymbol{\alpha})(p \cdot A) A_l A_m V \\
& + \sum_{l=1}^{3} \sum_{m=1}^{3} \sum_{n=1}^{3} p_l p_m p_n (p \cdot A) A_l A_m A_n \bigg) \frac{1}{p^2 + m_j^2 + \omega^2}.
\end{aligned} \tag{4.29}$$

The computation leading to this formula is tedious but elementary. In conclusion, setting $\mathcal{T}_{4,3}(\boldsymbol{A}) := \mathcal{T}_{4,3}^a(\boldsymbol{A}) + \mathcal{T}_{4,3}^b(\boldsymbol{A}) + \mathcal{T}_{4,3}^c(\boldsymbol{A})$, we have established that

$$T_{4,3}(\boldsymbol{A}) = \mathcal{T}_{4,3}(\boldsymbol{A}) + \mathcal{S}_{4,3}(\boldsymbol{A}), \tag{4.30}$$

where $\mathcal{T}_{4,3}(\boldsymbol{A})$ satisfies (4.28). Similarly, one can check that

$$T_{4,2}(\boldsymbol{A}) = \mathcal{T}_{4,2}(\boldsymbol{A}) + \mathcal{S}_{4,2}(\boldsymbol{A}), \tag{4.31}$$

with

$$\big\| \mathcal{T}_{4,2}(\boldsymbol{A}) \big\|_{\mathfrak{S}_1} \leq K \bigg(\sum_{j=0}^{2} \frac{|c_j|}{m_j} \bigg) \big\| \boldsymbol{A} \big\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}^4, \tag{4.32}$$

and

$$\begin{aligned}\mathcal{S}_{4,2}(\boldsymbol{A}) := \frac{2}{\pi}\int_{\mathbb{R}} \omega^2\, d\omega \sum_{j=0}^{2} c_j \frac{1}{(p^2+m_j^2+\omega^2)^3}\Big((p^2+m_j^2)\big(3|A|^2+3V^2 \\ -2(\boldsymbol{\alpha}\cdot A)\big)V^2 - 2(p\cdot\boldsymbol{\alpha}+m_j\boldsymbol{\beta})(p\cdot A)\big(3|A|^2+5V^2\big)V \\ +3\sum_{l=1}^{3} p_l (p\cdot A)A_l\big(|A|^2+5V^2-2(\boldsymbol{\alpha}\cdot A)V\big)\Big)\frac{1}{p^2+m_j^2+\omega^2}.\end{aligned} \tag{4.33}$$

Notice here again that the Kato-Seiler-Simon inequality implies that $\mathcal{S}_{4,2}(\boldsymbol{A})$ and $\mathcal{S}_{4,3}(\boldsymbol{A})$ are trace-class when $\boldsymbol{A} \in L^4(\mathbb{R}^3,\mathbb{R}^4)$ and conditions (2.7) are satisfied. Therefore, we always assume that $\boldsymbol{A} \in L^4(\mathbb{R}^3,\mathbb{R}^4)$ to make our calculations meaningful.

The last step in the proof is to compute the traces of the singular operators $\mathcal{S}_{4,1}(\boldsymbol{A})$, $\mathcal{S}_{4,2}(\boldsymbol{A})$ and $\mathcal{S}_{4,3}(\boldsymbol{A})$ for $\boldsymbol{A} \in L^4(\mathbb{R}^3,\mathbb{R}^4)$. As announced before we claim that

$$\operatorname{tr}\mathcal{S}_{4,1}(\boldsymbol{A}) - \operatorname{tr}\mathcal{S}_{4,2}(\boldsymbol{A}) + \operatorname{tr}\mathcal{S}_{4,3}(\boldsymbol{A}) = 0, \tag{4.34}$$

an identity which is enough to complete the proof of Lemma 4.4. To prove this we could make up an abstract argument based on gauge invariance. However we have to be careful with the fact that even if we can freely exchange the trace with the integration over ω, these only make sense *after* we have taken the sum over the coefficients c_j. The order matters and this complicates the mathematical analysis. Instead, we calculate the sum explicitly and verify that it is equal to 0.

A simple computation in Fourier space shows that

$$\begin{aligned}\operatorname{tr}\mathcal{S}_{4,1}(\boldsymbol{A}) = \frac{2}{\pi(2\pi)^{\frac{3}{2}}}\int_{\mathbb{R}^3} dp \int_{\mathbb{R}} \omega^2\, d\omega\Big(\sum_{j=0}^{2} c_j \frac{1}{(p^2+m_j^2+\omega^2)^3}\Big)\times \\ \times\int_{\mathbb{R}^3}\big(|A|^4+6|A|^2V^2+V^4\big).\end{aligned} \tag{4.35}$$

Similarly, one can check that

$$\begin{aligned}\operatorname{tr}\mathcal{S}_{4,2}(\boldsymbol{A}) =& \frac{8}{\pi(2\pi)^{\frac{3}{2}}}\int_{\mathbb{R}^3} dp \int_{\mathbb{R}} \omega^2\, d\omega\Big(\sum_{j=0}^{2} c_j \frac{1}{(p^2+m_j^2+\omega^2)^4}\Big)\times \\ &\times\Big(3\big(p^2+m_j^2\big)\int_{\mathbb{R}^3}\big(|A|^2V^2+V^4\big) \\ &+3\sum_{l=1}^{3}\sum_{m=1}^{3} p_l p_m \int_{\mathbb{R}^3}\big(A_lA_m|A|^2+5A_lA_mV^2\big)\Big).\end{aligned}$$

An integration by parts shows that

$$\int_{\mathbb{R}^3}\sum_{j=0}^{2} c_j \frac{p_l\, p_m\, dp}{(p^2+m_j^2+\omega^2)^4} = \frac{\delta_{l,m}}{6}\int_{\mathbb{R}^3}\sum_{j=0}^{2} c_j \frac{dp}{(p^2+m_j^2+\omega^2)^3},$$

and we obtain

$$\begin{aligned}
&\operatorname{tr}\mathcal{S}_{4,2}(\boldsymbol{A}) \\
&= \frac{24}{\pi(2\pi)^{\frac{3}{2}}}\int_{\mathbb{R}^3} dp \int_{\mathbb{R}} \omega^2\, d\omega \left(\sum_{j=0}^{2} c_j \frac{p^2+m_j^2}{(p^2+m_j^2+\omega^2)^4}\right) \int_{\mathbb{R}^3} \left(|A|^2V^2+V^4\right) \\
&+ \frac{4}{\pi(2\pi)^{\frac{3}{2}}}\int_{\mathbb{R}^3} dp \int_{\mathbb{R}} \omega^2\, d\omega \left(\sum_{j=0}^{2} c_j \frac{1}{(p^2+m_j^2+\omega^2)^3}\right) \int_{\mathbb{R}^3} \left(|A|^4+5|A|^2V^2\right).
\end{aligned} \tag{4.36}$$

Similar computations lead to the expression

$$\begin{aligned}
\operatorname{tr}\mathcal{S}_{4,3}(\boldsymbol{A}) &:= \frac{32}{\pi(2\pi)^{\frac{3}{2}}}\left(\int_{\mathbb{R}}\int_{\mathbb{R}^3}\sum_{j=0}^{2} c_j \frac{(p^2+m_j^2)^2\, dp\, \omega^2\, d\omega}{(p^2+m_j^2+\omega^2)^5}\right)\int_{\mathbb{R}^3} V^4 \\
&+\frac{8}{\pi(2\pi)^{\frac{3}{2}}}\left(\int_{\mathbb{R}}\int_{\mathbb{R}^3}\sum_{j=0}^{2} c_j \frac{dp\,\omega^2\, d\omega}{(p^2+m_j^2+\omega^2)^3}\Big(1+\frac{3(p^2+m_j^2)}{p^2+m_j^2+\omega^2}\Big)\right)\int_{\mathbb{R}^3}|A|^2V^2 \\
&+\frac{2}{\pi(2\pi)^{\frac{3}{2}}}\left(\int_{\mathbb{R}}\int_{\mathbb{R}^3}\sum_{j=0}^{2} c_j \frac{dp\,\omega^2\, d\omega}{(p^2+m_j^2+\omega^2)^3}\right)\int_{\mathbb{R}^3}|A|^4.
\end{aligned} \tag{4.37}$$

In view of (4.35) and (4.36), we obtain

$$\begin{aligned}
\operatorname{tr}\mathcal{S}_{4,1}(\boldsymbol{A}) - \operatorname{tr}\mathcal{S}_{4,2}(\boldsymbol{A}) + \operatorname{tr}\mathcal{S}_{4,3}(\boldsymbol{A}) &= \frac{2}{\pi(2\pi)^{\frac{3}{2}}}\left(\int_{\mathbb{R}^3} V^4\right)\int_{\mathbb{R}}\omega^2\, d\omega\int_{\mathbb{R}^3} dp\times \\
\times\sum_{j=0}^{2} c_j\left(\frac{1}{(p^2+m_j^2+\omega^2)^3} - 12\frac{p^2+m_j^2}{(p^2+m_j^2+\omega^2)^4} + 16\frac{(p^2+m_j^2)^2}{(p^2+m_j^2+\omega^2)^5}\right).&
\end{aligned}$$

A direct computation then shows that

$$\int_{\mathbb{R}}\left(\frac{1}{(1+\omega^2)^3} - \frac{12}{(1+\omega^2)^4} + \frac{16}{(1+\omega^2)^5}\right)\omega^2\, d\omega = 0.$$

This is enough to deduce (4.34), and complete the proof of Lemma 4.4. □

4.4. **Regularity of the sixth order term.** In this section, we come back to the sixth order term studied in the proof of Proposition 3.1. The sixth order term is defined as

$$\mathcal{R}_6(\boldsymbol{A}) = \frac{1}{4\pi}\int_{\mathbb{R}} \operatorname{tr}\left(R_6'(\omega,\boldsymbol{A}) + R_6'(-\omega,\boldsymbol{A})\right) d\omega, \tag{4.38}$$

where

$$R_6'(\omega,\boldsymbol{A}) := \sum_{j=0}^{2} c_j \frac{i\omega}{D_{m_j,\boldsymbol{A}}+i\omega}\Big(\big(\boldsymbol{\alpha}\cdot A - V\big)\frac{1}{D_{m_j,0}+i\omega}\Big)^6.$$

We have shown that it is trace-class when $\boldsymbol{A}\in \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$. We can indeed write estimate (3.14) as

$$\left\|\mathcal{R}_6(\boldsymbol{A})\right\|_{\mathfrak{S}_1} \le \frac{1}{2\pi}\int_{\mathbb{R}}\left\|R_6'(\omega,\boldsymbol{A})\right\|_{\mathfrak{S}_1} d\omega \le K\left(\sum_{j=0}^{2}\frac{|c_j|}{m_j^2}\right)\left\|\boldsymbol{A}\right\|^6_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}. \tag{4.39}$$

Here we want to prove that $\mathcal{R}_6$ is actually smooth, under suitable assumptions on $\boldsymbol{A}$. We first establish the continuity of $\mathcal{R}_6$ through

Lemma 4.5 (Continuity of the sixth order term)**.** *The functional $\mathcal{R}_6$ is locally θ–Hölder continuous on the space $\dot{H}^1_{\rm div}(\mathbb{R}^3)$ for any $0<\theta<1$.*

Proof. We consider the difference $R_6'(\omega,\boldsymbol{A})-R_6'(\omega,\boldsymbol{A}')$ for four-potentials $\boldsymbol{A}$ and $\boldsymbol{A}'$ in a given ball of $\dot{H}^1_{\rm div}(\mathbb{R}^3)$, which we write as

$$\begin{aligned}
&R_6'(\omega,\boldsymbol{A})-R_6'(\omega,\boldsymbol{A}')\\
&\quad=\sum_{j=0}^{2}c_j\bigg(i\omega\Big(\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}-\frac{1}{D_{m_j,\boldsymbol{A}'}+i\omega}\Big)\Big((\boldsymbol{\alpha}\cdot A-V)\frac{1}{D_{m_j,0}+i\omega}\Big)^6\\
&\quad+\sum_{k=0}^{5}\frac{i\omega}{D_{m_j,\boldsymbol{A}'}+i\omega}\Big((\boldsymbol{\alpha}\cdot A'-V')\frac{1}{D_{m_j,0}+i\omega}\Big)^k\times\\
&\quad\times\big(\boldsymbol{\alpha}\cdot(A-A')-V+V'\big)\frac{1}{D_{m_j,0}+i\omega}\Big((\boldsymbol{\alpha}\cdot A-V)\frac{1}{D_{m_j,0}+i\omega}\Big)^{5-k}\bigg).
\end{aligned}\tag{4.40}$$

The five terms in the sum over the index k can be estimated similarly as in the proof of (3.14). Their $\mathfrak{S}_1$–norms are bounded by a universal constant K times

$$\sum_{j=0}^{2}\frac{|c_j|}{(m_j^2+\omega^2)^{\frac{3}{2}}}\Big(\|\boldsymbol{A}\|^5_{\dot{H}^1_{\rm div}(\mathbb{R}^3)}+\|\boldsymbol{A}'\|^5_{\dot{H}^1_{\rm div}(\mathbb{R}^3)}\Big)\big\|\boldsymbol{A}-\boldsymbol{A}'\big\|_{\dot{H}^1_{\rm div}(\mathbb{R}^3)}.$$

If we follow the same proof for the first term, we need an estimate on the operator norm

$$\bigg\|i\omega\Big(\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}-\frac{1}{D_{m_j,\boldsymbol{A}'}+i\omega}\Big)\bigg\|.$$

On one hand, we remark that $\|(D_{m_j,\boldsymbol{A}}+i\omega)^{-1}\|\leq 1/\omega$, so that

$$\bigg\|i\omega\Big(\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}-\frac{1}{D_{m_j,\boldsymbol{A}'}+i\omega}\Big)\bigg\|\leq 2.\tag{4.41}$$

On the other hand, we can use the resolvent formula to write

$$\begin{aligned}
&\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}-\frac{1}{D_{m_j,\boldsymbol{A}'}+i\omega}\\
&\qquad=\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\big(\boldsymbol{\alpha}\cdot(\boldsymbol{A}-\boldsymbol{A}')+V'-V\big)\frac{1}{D_{m_j,\boldsymbol{A}'}+i\omega}.
\end{aligned}\tag{4.42}$$

For small $\boldsymbol{A}$, or small $\boldsymbol{A}'$, we have no problem in estimating this term using that the spectrum of $D_{m_j,\boldsymbol{A}}$ stays away from 0 by Lemma 2.1, and that $(D_{m_j,\boldsymbol{A}}+i\omega)^{-1}(D_{m_j,0}+i\omega)$ is bounded uniformly. The argument is essentially the same in the general case. We decompose the expression in the

right-hand side of (4.42) as

$$\begin{aligned} i\omega\Big(\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\big(\boldsymbol{\alpha}\cdot(\boldsymbol{A}-\boldsymbol{A}')+V'-V\big)\frac{1}{D_{m_j,\boldsymbol{A}'}+i\omega}\Big) \\ = \Big(\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\big(D_{m_j,\boldsymbol{A}}+i\mu\big)\Big)\times\Big(\frac{1}{D_{m_j,\boldsymbol{A}}+i\mu}\big(D_{m_j,0}+i\mu\big)\Big)\times \\ \times\Big(\frac{1}{D_{m_j,0}+i\mu}\big(\boldsymbol{\alpha}\cdot(\boldsymbol{A}-\boldsymbol{A}')+V'-V\big)\Big)\times\frac{i\omega}{D_{m_j,\boldsymbol{A}'}+i\omega}, \end{aligned} \tag{4.43}$$

for some positive number μ. We check that

$$\Big\|\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\big(D_{m_j,\boldsymbol{A}}+i\mu\big)\Big\| \leq \Big\|\frac{D_{m_j,\boldsymbol{A}}}{D_{m_j,\boldsymbol{A}}+i\omega}\Big\| + \Big\|\frac{i\mu}{D_{m_j,\boldsymbol{A}}+i\omega}\Big\| \leq 1+\frac{\mu}{|\omega|}. \tag{4.44}$$

Setting $\mu := 4K^2\|\boldsymbol{A}\|^2_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}$, we also remark that

$$\begin{aligned} \Big\|\frac{1}{D_{m_j,\boldsymbol{A}}+i\mu}(D_{m_j,0}+i\mu)\Big\| &= \Big\|\Big(1+\frac{1}{D_{m_j,0}+i\mu}\left(V-\boldsymbol{\alpha}\cdot A\right)\Big)^{-1}\Big\| \\ &\leq \sum_{n=0}^{\infty}\Big\|\frac{1}{D_{m_j,0}+i\mu}\left(V-\boldsymbol{\alpha}\cdot A\right)\Big\|^n \\ &\leq \sum_{n=0}^{\infty}\frac{K^n}{(m_j^2+\mu^2)^{\frac{n}{4}}}\|\boldsymbol{A}\|^n_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \leq 2. \end{aligned} \tag{4.45}$$

Recalling that $(i\omega)\|(D_{m_j,\boldsymbol{A}'}+i\omega)^{-1}\| \leq 1$, we infer from (4.42), (4.43), (4.44) and (4.45) that

$$\begin{aligned} \Big\|(i\omega)\Big(\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}-\frac{1}{D_{m_j,\boldsymbol{A}'}+i\omega}\Big)\Big\| \\ \leq &\frac{K}{\left(m_j^2+\mu^2\right)^{\frac{1}{4}}}\Big(1+\frac{\mu}{|\omega|}\Big)\|\boldsymbol{A}-\boldsymbol{A}'\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \\ \leq &K\Big(\frac{1}{\sqrt{m_j}}+\frac{1}{|\omega|}\|\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}\Big)\big\|\boldsymbol{A}-\boldsymbol{A}'\big\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}. \end{aligned} \tag{4.46}$$

In this bound, we can replace $\boldsymbol{A}$ by $\boldsymbol{A}'$ by symmetry. Recall that we are in a given ball in $\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$, so that $\|\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}$ is bounded by some constant.

Collecting estimates (4.41) and (4.46), we have shown that

$$\begin{aligned} &\int_{\mathbb{R}}\|R_6'(\omega,\boldsymbol{A})-R_6'(\omega,\boldsymbol{A}')\|_{\mathfrak{S}_1}\,d\omega \\ &\quad\leq K\Big(\sum_{j=0}^{2}\frac{|c_j|}{m_j^2}\Big)\Big(\|\boldsymbol{A}\|^5_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}+\|\boldsymbol{A}'\|^5_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}\Big)\big\|\boldsymbol{A}-\boldsymbol{A}'\big\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \\ &\quad+K\Big(\sum_{j=0}^{2}\frac{|c_j|}{m_j^2}\Big)\Big(\|\boldsymbol{A}\|^6_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}+\|\boldsymbol{A}'\|^6_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}\Big)\mathcal{I}(m_j,\boldsymbol{A},\boldsymbol{A}'), \end{aligned} \tag{4.47}$$

where

$$\mathcal{I}(m_j,\boldsymbol{A},\boldsymbol{A}') := \int_0^\infty \frac{d\omega}{(1+\omega^2)^{\frac{3}{2}}}\times \\ \times \min\Big\{2,\ \Big(\frac{1}{\sqrt{m_j}}+\frac{1}{m_j\omega}\|\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}\Big)\big\|\boldsymbol{A}-\boldsymbol{A}'\big\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}\Big\}.$$

Assuming that $\|\boldsymbol{A}-\boldsymbol{A}'\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \leq m_j/(\sqrt{m_j}+\|\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)})$ for any $j=0,1,2$, we can estimate the integral $\mathcal{I}(m_j,\boldsymbol{A},\boldsymbol{A}')$ as

$$\big|\mathcal{I}(m_j,\boldsymbol{A},\boldsymbol{A}')\big| \leq \frac{1}{\sqrt{m_j}}\Big(\int_0^\infty \frac{d\omega}{(1+\omega^2)^{\frac{3}{2}}}\Big)\big\|\boldsymbol{A}-\boldsymbol{A}'\big\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \\ + 2\mathcal{J}\Big(\frac{1}{2m_j}\|\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}\|\boldsymbol{A}-\boldsymbol{A}'\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}\Big),$$

with

$$\mathcal{J}(t) := \int_0^t \frac{d\omega}{(1+\omega^2)^{\frac{3}{2}}} + t\int_t^\infty \frac{d\omega}{\omega(1+\omega^2)^{\frac{3}{2}}}.$$

It remains to observe that

$$\mathcal{J}(t) \leq Kt\big(1+|\log t|\big),$$

and to combine with (4.38) and (4.47), to conclude that the functional $\mathcal{R}_6$ is locally θ–Hölder for any $0<\theta<1$. □

We next turn to the differentiability of $\mathcal{R}_6$.

Lemma 4.6 (Regularity of the sixth order term)**.** *The functional $\mathcal{R}_6$ is of class $\mathcal{C}^\infty$ on the open subset $\mathcal{H}$ of $\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$ containing all the four-potentials $\boldsymbol{A}$ such that $0\notin\sigma(D_{m_j,\boldsymbol{A}})$ for each $j=0,1,2$. Moreover, there exists a universal constant K such that*

$$\big\|\mathrm{d}^2\mathcal{R}_6(\boldsymbol{A})\big\| \leq K\sum_{j=0}^2 \frac{|c_j|}{m_j^2}\Big(1+\frac{L_{\boldsymbol{A}}^2}{m_j}\|\boldsymbol{A}\|^2_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}\Big)\big\|\boldsymbol{A}\big\|^4_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}, \tag{4.48}$$

where

$$L_{\boldsymbol{A}} := \max\big\{\|(D_{m_j,\boldsymbol{A}}+i\omega)^{-1}(D_{m_j,0}+i\omega)\|,\ \omega\in\mathbb{R},\ j=0,1,2\big\} < \infty.$$

Proof. The proof relies on elements in the proof of Lemma 4.5. When 0 is not an eigenvalue of $D_{m_j,\boldsymbol{A}}$ for each $j=0,1,2$, we can deduce from Lemma 2.1 the existence of a positive constant $K_{\boldsymbol{A}}$ such that

$$\Big\|\frac{1}{D_{m_j,\boldsymbol{A}'}+i\omega}\Big\| \leq \min\Big\{K_{\boldsymbol{A}},\frac{1}{|\omega|}\Big\}, \tag{4.49}$$

for any $\boldsymbol{A}'\in\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$, with $\|\boldsymbol{A}'-\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}$ small enough. As a consequence, we can replace estimate (4.44) by the inequality

$$\Big\|\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\big(D_{m_j,\boldsymbol{A}}+i\mu\big)\Big\| \leq 1+K_{\boldsymbol{A}}\mu.$$

Since

$$\begin{aligned}\Big\|\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\big(D_{m_j,0}+i\omega\big)\Big\| \\ \leq \Big\|\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\big(D_{m_j,0}+i\mu\big)\Big\| + |\omega-\mu|\min\Big\{K_{\boldsymbol{A}},\frac{1}{|\omega|}\Big\},\end{aligned}$$

it follows that

$$\begin{aligned}&\Big\|\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\big(D_{m_j,0}+i\omega\big)\Big\| \\ &\quad\leq \big(1+K_{\boldsymbol{A}}\mu\big)\Big\|\frac{1}{D_{m_j,\boldsymbol{A}}+i\mu}\big(D_{m_j,0}+i\mu\big)\Big\| + |\omega-\mu|\min\Big\{K_{\boldsymbol{A}},\frac{1}{|\omega|}\Big\}.\end{aligned} \tag{4.50}$$

Following the lines of the proof of (4.45), we deduce that the quantity in the right-hand side of (4.50) is bounded independently on ω by a positive constant $L_{\boldsymbol{A}}$, depending only on the four-potential $\boldsymbol{A}$ and the mass m_j. Actually, we can claim, up to a possible larger choice of $L_{\boldsymbol{A}}$, that

$$\Big\|\frac{1}{D_{m_j,\boldsymbol{A}'}+i\omega}\big(D_{m_j,0}+i\omega\big)\Big\| \leq L_{\boldsymbol{A}},$$

for any $\omega\in\mathbb{R}$, $j=0,1,2$, and $\boldsymbol{A}'\in\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$, with $\|\boldsymbol{A}'-\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}$ small enough.

As a result, we can upgrade (4.46) into

$$\Big\|i\omega\Big(\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}-\frac{1}{D_{m_j,\boldsymbol{A}'}+i\omega}\Big)\Big\| \leq \frac{KL_{\boldsymbol{A}}}{(m_j^2+\omega^2)^{\frac{1}{4}}}\big\|\boldsymbol{A}-\boldsymbol{A}'\big\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}.$$

Similarly, we can compute

$$\begin{aligned}\Big\|\frac{i\omega}{D_{m_j,\boldsymbol{A}}+i\omega}\big(\boldsymbol{\alpha}\cdot(\boldsymbol{A}-\boldsymbol{A}')+V'-V\big)\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\Big\| \\ \leq \frac{KL_{\boldsymbol{A}}}{(m_j^2+\omega^2)^{\frac{1}{4}}}\big\|\boldsymbol{A}-\boldsymbol{A}'\big\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)}.\end{aligned} \tag{4.51}$$

At this stage, we can iterate the resolvent expansion in (4.42) to obtain

$$\begin{aligned}&\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}-\frac{1}{D_{m_j,\boldsymbol{A}'}+i\omega} \\ &\qquad=\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\big(\boldsymbol{\alpha}\cdot(\boldsymbol{A}-\boldsymbol{A}')+V'-V\big)\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega} \\ &\qquad+\Big(\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\big(\boldsymbol{\alpha}\cdot(\boldsymbol{A}-\boldsymbol{A}')+V'-V\big)\Big)^2\frac{1}{D_{m_j,\boldsymbol{A}'}+i\omega}.\end{aligned}$$

Inserting this identity into (4.40), we can write

$$R_6'(\omega,\boldsymbol{A})-R_6'(\omega,\boldsymbol{A}')=\mathrm{d}_{\boldsymbol{A}}R_6'(\omega,\boldsymbol{A})(\boldsymbol{A}-\boldsymbol{A}')+r_6'\big(\omega,\boldsymbol{A},\boldsymbol{A}'\big). \tag{4.52}$$

Here, $\mathrm{d}_{\boldsymbol{A}} R_6'(\omega, \boldsymbol{A})$ refers to the continuous linear mapping from $\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$ to $\mathfrak{S}_1(\mathbb{R}^3, \mathbb{R}^4)$ given by

$$\begin{aligned}
&\mathrm{d}_{\boldsymbol{A}} R_6'(\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) \\
&= \sum_{j=0}^{2} c_j \Big(\frac{i\omega}{D_{m_j,\boldsymbol{A}} + i\omega} (\boldsymbol{\alpha}\cdot\mathfrak{a} - \mathfrak{v}) \frac{1}{D_{m_j,\boldsymbol{A}} + i\omega} \Big((\boldsymbol{\alpha}\cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big)^6 \\
&+ \sum_{k=0}^{5} \frac{i\omega}{D_{m_j,\boldsymbol{A}} + i\omega} \Big((\boldsymbol{\alpha}\cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big)^{5-k} \Big((\boldsymbol{\alpha}\cdot\mathfrak{a} - \mathfrak{v}) \frac{1}{D_{m_j,0} + i\omega} \Big) \times \\
&\qquad \times \Big((\boldsymbol{\alpha}\cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big)^k \Big).
\end{aligned} \tag{4.53}$$

In view of (4.51), and again the computations in the proof of estimate (3.14), the operator norm of $\mathrm{d}_{\boldsymbol{A}} R_6'(\omega, \boldsymbol{A})$ is indeed bounded by

$$\begin{aligned}
&\big\| \mathrm{d}_{\boldsymbol{A}} R_6'(\omega, \boldsymbol{A}) \big\| \\
&\qquad \leq K \sum_{j=0}^{2} \frac{|c_j|}{(m_j^2 + \omega^2)^{\frac{3}{2}}} \|\boldsymbol{A}\|^5_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \Big(1 + \frac{L_{\boldsymbol{A}}}{(m_j^2 + \omega^2)^{\frac{1}{4}}} \|\boldsymbol{A}\|_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \Big).
\end{aligned} \tag{4.54}$$

Similarly, the remainder $r_6'\big(\omega, \boldsymbol{A}, \boldsymbol{A}'\big)$ in (4.52) may be estimated as

$$\begin{aligned}
&\Big\| r_6'\big(\omega, \boldsymbol{A}, \boldsymbol{A}'\big) \Big\|_{\mathfrak{S}_1} \\
&\quad \leq K \|\boldsymbol{A} - \boldsymbol{A}'\|^2_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \sum_{j=0}^{2} \frac{|c_j|}{(m_j^2 + \omega^2)^{\frac{3}{2}}} \big(\|\boldsymbol{A}\|^4_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} + \|\boldsymbol{A}'\|^4_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \big) \times \\
&\qquad \times \Big(1 + \frac{L_{\boldsymbol{A}}^2}{(m_j^2 + \omega^2)^{\frac{1}{2}}} \big(\|\boldsymbol{A}\|^2_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} + \|\boldsymbol{A}'\|^2_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \big) \Big).
\end{aligned} \tag{4.55}$$

Collecting (4.38), (4.52), (4.54) and (4.55) is enough to establish the continuous differentiability of the function $\mathcal{R}_6$ on a neighborhood of $\boldsymbol{A}$, with a differential given by

$$\mathrm{d}\mathcal{R}_6(\boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) = \frac{1}{4\pi} \int_{\mathbb{R}} \mathrm{tr} \Big(\mathrm{d}_{\boldsymbol{A}} R_6'(\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) + \mathrm{d}_{\boldsymbol{A}} R_6'(-\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) \Big) \, d\omega. \tag{4.56}$$

Finally, we can extend the previous arguments for the continuous differentiability of $\mathcal{R}_6$ to the proof that it is actually of class $\mathcal{C}^\infty$. In particular, we can check that the norm of the quadratic form $\mathrm{d}^2_{\boldsymbol{A}} R_6'$ is bounded by

$$\begin{aligned}
&\Big\| \mathrm{d}^2_{\boldsymbol{A}} R_6'\big(\omega, \boldsymbol{A}\big) \Big\| \\
&\qquad \leq K \sum_{j=0}^{2} \frac{|c_j|}{(m_j^2 + \omega^2)^{\frac{3}{2}}} \|\boldsymbol{A}\|^4_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \Big(1 + \frac{L_{\boldsymbol{A}}^2}{(m_j^2 + \omega^2)^{\frac{1}{2}}} \|\boldsymbol{A}\|^2_{\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)} \Big).
\end{aligned}$$

Estimate (4.48) follows integrating with respect to ω. □

When $\|\boldsymbol{A}\|_{\dot{H}^1_{\rm div}(\mathbb{R}^3)}$ is small enough, we can prove that the constant $L_{\boldsymbol{A}}$ does not depend on $\boldsymbol{A}$.

Corollary 4.1 (Estimate in a neighborhood of zero)**.** *Assume that c_j and m_j satisfy* (2.10)*. There exists a universal constant η such that, given any $\boldsymbol{A} \in \dot{H}^1_{\rm div}(\mathbb{R}^3)$ with $\|\boldsymbol{A}\|_{\dot{H}^1_{\rm div}(\mathbb{R}^3)} \leq \eta\sqrt{m_0}$, the functional $\mathcal{R}_6$ is of class $\mathcal{C}^\infty$ on the ball*

$$\mathcal{B}_{\boldsymbol{A}}(\eta\sqrt{m_0}) = \left\{\boldsymbol{A} \in \dot{H}^1_{\rm div}(\mathbb{R}^3) \ : \ \|\boldsymbol{A}\|_{\dot{H}^1_{\rm div}(\mathbb{R}^3)} \leq \eta\sqrt{m_0}\right\},$$

and satisfies the estimate

$$\left\|{\rm d}^2\mathcal{R}_6(\boldsymbol{A})\right\| \leq K\left(\sum_{j=0}^{2}\frac{|c_j|}{m_j^2}\right)\|\boldsymbol{A}\|^4_{\dot{H}^1_{\rm div}(\mathbb{R}^3)}. \tag{4.57}$$

Proof. When $\boldsymbol{A}$ is small enough, the spectrum of $D_{m_j,\boldsymbol{A}}$ does not contain 0 by Lemma 2.1. Moreover, when

$$\|\boldsymbol{A}\|_{\dot{H}^1_{\rm div}(\mathbb{R}^3)} \leq \eta\min\left\{\sqrt{m_0},\sqrt{m_1},\sqrt{m_2}\right\} = \eta\sqrt{m_0},$$

for η small enough, we can infer from (4.45) that

$$L_{\boldsymbol{A}} \leq 2.$$

Inserting in (4.48), and using the inequality $\|\boldsymbol{A}\|_{\dot{H}^1_{\rm div}(\mathbb{R}^3)} \leq \eta\sqrt{m_j}$, gives estimate (4.57). □

5. Proof of Theorem 2.1

With the results of the previous section at hand, the proof of Theorem 2.1 is only a few lines. As a matter of fact, given any $\boldsymbol{A} \in L^1(\mathbb{R}^3,\mathbb{R}^4)\cap\dot{H}^1_{\rm div}(\mathbb{R}^3)$, we have shown that the functional $\mathcal{F}_{\rm PV}(\boldsymbol{A})$ is well-defined by the expression

$$\mathcal{F}_{\rm PV}(\boldsymbol{A}) = \mathcal{F}_2(\boldsymbol{F}) + \mathcal{R}(\boldsymbol{A}), \tag{5.1}$$

where

$$\mathcal{F}_2(\boldsymbol{F}) := {\rm tr}\left({\rm tr}_{\mathbb{C}^4}\,T_2(\boldsymbol{A})\right),$$

and

$$\mathcal{R}(\boldsymbol{A}) := {\rm tr}\left({\rm tr}_{\mathbb{C}^4}\,T_4(\boldsymbol{A})\right) + {\rm tr}\left({\rm tr}_{\mathbb{C}^4}\,T_6'(\boldsymbol{A})\right),$$

are defined in (4.1). By Lemma 4.2, the function $\mathcal{F}_2$ is given by (2.15) and it is quadratic with respect to $\boldsymbol{F}$. Since M is bounded, we deduce that $\mathcal{F}_2$ is smooth on $L^2(\mathbb{R}^3,\mathbb{R}^6)$. On the other hand, the function $\boldsymbol{A} \mapsto \mathcal{F}_4(\boldsymbol{A}) := {\rm tr}({\rm tr}_{\mathbb{C}^4}\,T_4(\boldsymbol{A}))$ is quartic and satisfies (4.19). Hence, it is a smooth function on $\dot{H}^1_{\rm div}(\mathbb{R}^3)$. We have proved separately in Lemma 4.5 above that $\mathcal{R}_6(\boldsymbol{A}) = {\rm tr}({\rm tr}_{\mathbb{C}^4}\,T_6'(\boldsymbol{A}))$ is an Hölder continuous function on $\dot{H}^1_{\rm div}(\mathbb{R}^3)$, which satisfies (3.14). We deduce from all this that $\mathcal{F}_{\rm PV}$ has a unique continuous extension to $\dot{H}^1_{\rm div}(\mathbb{R}^3)$, which is given by (5.1), and that $\mathcal{R}$ satisfies estimate (2.14). The properties of M can be found in Lemma 4.3.

6. Proof of Theorem 2.2

In view of the results in Sections 3 and 4, the functional $\mathcal{F}_{\rm PV}$ is smooth on the open subset $\mathcal{H}$ of $\dot{H}^1_{\rm div}(\mathbb{R}^3)$ containing all the four-potentials $\boldsymbol{A}$ such that $0 \notin \sigma(D_{m_j,\boldsymbol{A}})$ for each $j = 0, 1, 2$. Indeed, the function $\boldsymbol{A} \mapsto \mathcal{F}_4(\boldsymbol{A}) := \mathrm{tr}(\mathrm{tr}_{\mathbb{C}^4} T_4(\boldsymbol{A}))$ is quartic and satisfies (4.19). Hence, it is of class $\mathcal{C}^\infty$ on $\dot{H}^1_{\rm div}(\mathbb{R}^3)$. Similarly, in view of Lemmas 4.2 and 4.3, the quadratic map $\mathcal{F}_2$ is smooth on $L^2(\mathbb{R}^3, \mathbb{R}^6)$. On the other hand, we have shown in Section 4.4 that $\mathcal{R}_6$ is smooth when 0 is not an eigenvalue of $D_{m_j,\boldsymbol{A}}$ for $j = 0, 1, 2$. We deduce that $\mathcal{F}_{\rm PV}$ is smooth on the set $\mathcal{H}$.

In order to complete the proof of Theorem 2.2, it remains to identify $\mathrm{d}\mathcal{F}_{\rm PV}(\boldsymbol{A})$. As mentioned in Formulas (2.19) and (2.20), this differential is related to the operator

$$Q_{\boldsymbol{A}} := \sum_{j=0}^{2} c_j \, \mathbb{1}_{(-\infty,0)}\big(D_{m_j,\boldsymbol{A}}\big).$$

Concerning the properties of the operator $Q_{\boldsymbol{A}}$, we can establish the following

Lemma 6.1 (Properties of $\rho_{\boldsymbol{A}}$ and $j_{\boldsymbol{A}}$)**.** *Assume that c_j and m_j satisfy conditions* (2.10)*.*

(i) Let $\boldsymbol{A} \in \dot{H}^1_{\rm div}(\mathbb{R}^3)$ be a four-potential such that 0 is not an eigenvalue of $D_{m_j,\boldsymbol{A}}$ for $j = 0, 1, 2$. Then the operators $\mathrm{tr}_{\mathbb{C}^4}\, Q_{\boldsymbol{A}}$ and $\mathrm{tr}_{\mathbb{C}^4}\, \boldsymbol{\alpha} Q_{\boldsymbol{A}}$ are locally trace-class on $L^2(\mathbb{R}^3, \mathbb{R}^4)$. More precisely, given any function $\chi \in L^\infty_c(\mathbb{R}^3)$ (that is, bounded with compact support), the maps

$$\boldsymbol{A} \in \mathcal{H} \mapsto \chi\big(\mathrm{tr}_{\mathbb{C}^4}\, Q_{\boldsymbol{A}}\big)\chi \in \mathfrak{S}_1$$

and

$$\boldsymbol{A} \in \mathcal{H} \mapsto \chi\big(\mathrm{tr}_{\mathbb{C}^4}\, \boldsymbol{\alpha}\, Q_{\boldsymbol{A}}\big)\chi \in \mathfrak{S}_1$$

are continuous from $\mathcal{H}$ to $\mathfrak{S}_1$. In particular, the density $\rho_{\boldsymbol{A}}$ and the current $j_{\boldsymbol{A}}$, given by

$$\rho_{\boldsymbol{A}}(x) := \big[\mathrm{tr}_{\mathbb{C}^4}\, Q_{\boldsymbol{A}}\big](x,x) \quad \text{and} \quad j_{\boldsymbol{A}}(x) := \big[\mathrm{tr}_{\mathbb{C}^4}\, \boldsymbol{\alpha}\, Q_{\boldsymbol{A}}\big](x,x),$$

are well-defined and locally integrable on $\mathbb{R}^3$. Moreover, the maps $\boldsymbol{A} \mapsto \rho_{\boldsymbol{A}}\, \chi^2$ and $\boldsymbol{A} \mapsto j_{\boldsymbol{A}}\, \chi^2$ are continuous from $\mathcal{H}$ to $L^1(\mathbb{R}^3)$. Finally, for $\boldsymbol{A} \equiv 0$, we have

$$\rho_0 \equiv 0 \quad \text{and} \quad j_0 \equiv 0.$$

(ii) If moreover $\boldsymbol{A} \in L^1(\mathbb{R}^3, \mathbb{R}^4)$, then, the operators $\mathrm{tr}_{\mathbb{C}^4}\,(Q_{\boldsymbol{A}} - Q_0)$ and $\mathrm{tr}_{\mathbb{C}^4}\, \boldsymbol{\alpha}(Q_{\boldsymbol{A}} - Q_0)$ are trace-class on $L^2(\mathbb{R}^3, \mathbb{R}^4)$, and the density $\rho_{\boldsymbol{A}}$ and the current $j_{\boldsymbol{A}}$ are in $L^1(\mathbb{R}^3)$.

Proof. We split the proof into three steps. First, we consider the special case $\boldsymbol{A} \equiv 0$.

The operators $\mathrm{tr}_{\mathbb{C}^4}\, Q_0$ and $\mathrm{tr}_{\mathbb{C}^4}\, \boldsymbol{\alpha} Q_0$ are locally trace-class. Using that $\sum_{j=0}^{2} c_j = 0$, we can write

$$Q_0 = \sum_{j=0}^{2} c_j \left(\mathbb{1}_{(-\infty,0)}\big(D_{m_j,0}\big) - \frac{1}{2}\right) = -\frac{1}{2}\,\mathrm{tr}_{\mathbb{C}^4} \sum_{j=0}^{2} c_j \, \frac{D_{m_j,0}}{|D_{m_j,0}|}.$$

As a consequence, we obtain

$$\operatorname{tr}_{\mathbb{C}^4} Q_0 = 0.$$

In particular, the density ρ_0 is well-defined and it identically vanishes on $\mathbb{R}^3$. Similarly, we have

$$\operatorname{tr}_{\mathbb{C}^4} \boldsymbol{\alpha} Q_0 = -2 \sum_{j=0}^{2} c_j \, \frac{p}{(p^2+m_j^2)^{\frac{1}{2}}}.$$

Due to conditions (2.7), the latter function behaves like

$$\sum_{j=0}^{2} c_j \, \frac{p}{(p^2+m_j^2)^{\frac{1}{2}}} \sim \frac{3}{8} \sum_{j=0}^{2} c_j \, m_j^4 \, \frac{p}{|p|^5},$$

as $|p| \to \infty$, hence it is in $L^1(\mathbb{R}^3)$. By the Kato-Seiler-Simon inequality (2.5), we deduce that the operator $\operatorname{tr}_{\mathbb{C}^4} \boldsymbol{\alpha} \chi Q_0 \chi$ is trace-class for any $\chi \in L^2(\mathbb{R}^3)$. Hence, $\operatorname{tr}_{\mathbb{C}^4} \boldsymbol{\alpha} Q_0$ is locally trace-class. In particular, the current j_0 is well-defined and locally integrable on $\mathbb{R}^3$. Moreover, we can compute

$$\begin{aligned} \int_{\mathbb{R}^3} j_0 \, \chi^2 &= \operatorname{tr}\left(\operatorname{tr}_{\mathbb{C}^4} \boldsymbol{\alpha} \chi Q_0 \chi \right) \\ &= -\frac{1}{4\pi^3} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \sum_{j=0}^{2} c_j \, \frac{p}{(p^2+m_j^2)^{\frac{1}{2}}} |\widehat{\chi}(q-p)|^2 \, dp \, dq, \end{aligned}$$

which shows that

$$j_0 = -\frac{1}{4\pi^3} \int_{\mathbb{R}^3} \sum_{j=0}^{2} c_j \, \frac{p}{(p^2+m_j^2)^{\frac{1}{2}}} \, dp = 0$$

by rotational symmetry.

We next consider the general case.

The operators $\operatorname{tr}_{\mathbb{C}^4} Q_{\boldsymbol{A}}$ and $\operatorname{tr}_{\mathbb{C}^4} \boldsymbol{\alpha} Q_{\boldsymbol{A}}$ are (locally) trace-class. From the previous discussion, we conclude that it is sufficient to prove that the operators $\operatorname{tr}_{\mathbb{C}^4}(Q_{\boldsymbol{A}} - Q_0)$ and $\operatorname{tr}_{\mathbb{C}^4} \boldsymbol{\alpha}(Q_{\boldsymbol{A}} - Q_0)$ are locally trace-class. The corresponding charge and current densities will be the same as that of $Q_{\boldsymbol{A}}$.

Concerning the (local) trace-class nature of the operator $Q_{\boldsymbol{A}} - Q_0$, we follow the proof of Proposition 3.1. Our starting point is the integral formula

$$\operatorname{sign} x = \frac{2}{\pi} \int_{\mathbb{R}} \frac{x \, \omega^2}{(x^2+\omega^2)^2} \, d\omega = \frac{1}{2\pi} \int_{\mathbb{R}} \Big(\frac{i\omega}{(x+i\omega)^2} - \frac{i\omega}{(x-i\omega)^2} \Big) \, d\omega. \quad (6.1)$$

When T is a self-adjoint operator on $L^2(\mathbb{R}^3, \mathbb{R}^4)$ with domain $D(T)$, we deduce that the sign of T is given by

$$\operatorname{sign} T = \frac{1}{2\pi} \int_{\mathbb{R}} \Big(\frac{i\omega}{(T+i\omega)^2} - \frac{i\omega}{(T-i\omega)^2} \Big) \, d\omega, \quad (6.2)$$

the integral in the right-hand side of (6.2) being convergent as an operator from $D(T)$ to $L^2(\mathbb{R}^3, \mathbb{C}^4)$.

In particular, the operator

$$Q_{\boldsymbol{A}} - Q_0 = -\frac{1}{2} \sum_{j=0}^{2} c_j \left(\operatorname{sign} D_{m_j, \boldsymbol{A}} - \operatorname{sign} D_{m_j, 0} \right),$$

is given by the expression

$$Q_{\boldsymbol{A}} - Q_0 = -\frac{1}{4\pi}\int_{\mathbb{R}} \sum_{j=0}^{2} c_j \Big(\frac{i\omega}{(D_{m_j,\boldsymbol{A}} + i\omega)^2} - \frac{i\omega}{(D_{m_j,0} + i\omega)^2} - \frac{i\omega}{(D_{m_j,\boldsymbol{A}} - i\omega)^2} + \frac{i\omega}{(D_{m_j,0} - i\omega)^2} \Big)\, d\omega, \tag{6.3}$$

on $H^1(\mathbb{R}^3, \mathbb{C}^4)$. In order to establish statements (ii) and (iii) of Lemma 6.1, we will prove that

$$\int_{\mathbb{R}} \Big\| \sum_{j=0}^{2} c_j \ \mathrm{tr}_{\mathbb{C}^4}\, \mathfrak{m}\, \chi \Big(\frac{i\omega}{(D_{m_j,\boldsymbol{A}} + i\omega)^2} - \frac{i\omega}{(D_{m_j,0} + i\omega)^2} - \frac{i\omega}{(D_{m_j,\boldsymbol{A}} - i\omega)^2} + \frac{i\omega}{(D_{m_j,0} - i\omega)^2} \Big) \chi \Big\|_{\mathfrak{S}_1} d\omega < \infty, \tag{6.4}$$

for any of the matrices $\mathfrak{m} = I_4, \boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \boldsymbol{\alpha}_3$, and either when $\boldsymbol{A} \in L^1(\mathbb{R}^3, \mathbb{R}^4) \cap H^1(\mathbb{R}^3, \mathbb{R}^4)$ and $\chi \equiv 1$, or when $\boldsymbol{A} \in \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$ and $\chi \in L^\infty_c(\mathbb{R}^3, \mathbb{R})$. In the different cases, the $\mathbb{C}^4$–traces of the operators $\mathfrak{m}(Q_{\boldsymbol{A}} - Q_0)$, respectively $\mathfrak{m}\chi(Q_{\boldsymbol{A}} - Q_0)\chi$, will define trace-class operators on $L^2(\mathbb{R}^3, \mathbb{C}^4)$. Then the operators $\mathrm{tr}_{\mathbb{C}^4}\, \mathfrak{m} Q_{\boldsymbol{A}}$ will be locally trace-class and the density $\rho_{\boldsymbol{A}}$ and the current $j_{\boldsymbol{A}}$ will be well-defined and locally integrable on $\mathbb{R}^3$. Moreover, they will be integrable on $\mathbb{R}^3$ for any $\boldsymbol{A} \in L^1(\mathbb{R}^3, \mathbb{R}^4) \cap H^1(\mathbb{R}^3, \mathbb{R}^4)$.

In order to prove (6.4), we use the expansion

$$\begin{aligned} &\frac{i\omega}{(D_{m_j,\boldsymbol{A}} + i\omega)^2} - \frac{i\omega}{(D_{m_j,0} + i\omega)^2} - \frac{i\omega}{(D_{m_j,\boldsymbol{A}} - i\omega)^2} + \frac{i\omega}{(D_{m_j,0} - i\omega)^2} \\ &\qquad := \sum_{n=1}^{5} \Big(Q_n(\omega, \boldsymbol{A}) + Q_n(-\omega, \boldsymbol{A}) \Big) + Q'_6(\omega, \boldsymbol{A}) + Q'_6(-\omega, \boldsymbol{A}) \\ &\qquad\qquad - Q'_7(\omega, \boldsymbol{A}) - Q'_7(-\omega, \boldsymbol{A}), \end{aligned} \tag{6.5}$$

with

$$Q_n(\omega, \boldsymbol{A}) := (n+1) \sum_{j=0}^{2} c_j \, \frac{i\omega}{(D_{m_j,0} + i\omega)^2} \Big((\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big)^n,$$

$$Q'_6(\omega, \boldsymbol{A}) := 7 \sum_{j=0}^{2} c_j \, \frac{i\omega}{(D_{m_j,\boldsymbol{A}} + i\omega)^2} \Big((\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big)^6,$$

and

$$Q'_7(\omega, \boldsymbol{A}) := 6 \sum_{j=0}^{2} c_j \, \frac{i\omega}{(D_{m_j,\boldsymbol{A}} + i\omega)^2} \Big((\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0} + i\omega} \Big)^7.$$

We next estimate the terms related to the operators $Q_n(\omega, \boldsymbol{A})$, $Q'_6(\omega, \boldsymbol{A})$ and $Q'_7(\omega, \boldsymbol{A})$, as we have previously done for the operators $R_n(\omega, \boldsymbol{A})$ and $R'_6(\omega, \boldsymbol{A})$ in Section 3.

Concerning $Q'_6(\omega, \boldsymbol{A})$ and $Q'_7(\omega, \boldsymbol{A})$, we recall that 0 is not an eigenvalue of $D_{m_j,\boldsymbol{A}}$ for each $j = 0, 1, 2$. Hence, there exists a positive constant K such

that

$$\Big\| \frac{1}{D_{m_j,\boldsymbol{A}} + i\omega} \Big\| \leq K, \tag{6.6}$$

for all $\omega \in \mathbb{R}$ and $j = 0, 1, 2$. Following the proof of (3.14), we deduce that

$$\begin{aligned} \int_{\mathbb{R}} \big(\|Q_6'(\omega, \boldsymbol{A})\|_{\mathfrak{S}_1} + \|Q_7'(\omega, \boldsymbol{A})\|_{\mathfrak{S}_1} \big)\, d\omega \\ \leq K \sum_{j=0}^{2} \frac{|c_j|}{m_j^2} \|\nabla \boldsymbol{A}\|_{L^2}^6 \left(1 + \frac{1}{\sqrt{m_j}} \|\nabla \boldsymbol{A}\|_{L^2} \right). \end{aligned}$$

As a consequence, the integrals

$$\mathcal{Q}_6'(\boldsymbol{A}) := \frac{1}{4\pi} \int_{\mathbb{R}} \big(Q_6'(\omega, \boldsymbol{A}) + Q_6'(-\omega, \boldsymbol{A}) \big)\, d\omega,$$

and

$$\mathcal{Q}_7'(\boldsymbol{A}) := \frac{1}{4\pi} \int_{\mathbb{R}} \big(Q_7'(\omega, \boldsymbol{A}) + Q_7'(-\omega, \boldsymbol{A}) \big)\, d\omega,$$

define trace-class operators on $L^2(\mathbb{R}^3, \mathbb{R}^4)$ when $\boldsymbol{A} \in \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$. The related densities $\rho_6'(\boldsymbol{A})$ and $\rho_7'(\boldsymbol{A})$, and currents $j_6'(\boldsymbol{A})$ and $j_7'(\boldsymbol{A})$, are well-defined and integrable on $\mathbb{R}^3$. Moreover, in view of (6.6), we can repeat the arguments in the proof of Lemma 4.6 in order to establish the smoothness of the maps $\boldsymbol{A} \mapsto \mathcal{Q}_6'(\boldsymbol{A})$ and $\boldsymbol{A} \mapsto \mathcal{Q}_7'(\boldsymbol{A})$ from $\mathcal{H}$ onto $\mathfrak{S}_1$.

For $3 \leq n \leq 5$, the operators $Q_n(\omega, \boldsymbol{A})$ satisfy the estimates

$$\int_{\mathbb{R}} \big\| Q_n(\omega, \boldsymbol{A}) \big\|_{\mathfrak{S}_1} d\omega \leq K_n \big\| \boldsymbol{A} \big\|_{L^n}^n, \tag{6.7}$$

and

$$\int_{\mathbb{R}} \big\| \chi Q_n(\omega, \boldsymbol{A}) \chi \big\|_{\mathfrak{S}_1} d\omega \leq K_n \big\| \boldsymbol{A} \big\|_{L^6}^n \big\| \chi \big\|_{L^{\frac{12}{6-n}}}^2, \tag{6.8}$$

for any function $\chi \in L^\infty_c(\mathbb{R}^3)$. Here, K_n refers to a positive constant depending only on the coefficients c_j and the masses m_j. For $n = 4$ and $n = 5$, we can indeed use the Kato-Seiler-Simon inequality (2.5) to write

$$\big\| Q_n(\omega, \boldsymbol{A}) \big\|_{\mathfrak{S}_1} \leq K \sum_{j=0}^{2} |c_j| \, \big\| \boldsymbol{A} \big\|_{L^n}^n \int_{\mathbb{R}^3} \frac{|\omega|\, dp}{(p^2 + m_j^2 + \omega^2)^{\frac{n+2}{2}}}.$$

Integrating with respect to ω, we obtain inequality (6.7) with

$$K_n := K \sum_{j=0}^{2} \frac{|c_j|}{m_j^{n-3}}.$$

For $n = 3$, we rely on the identity $c_0 + c_1 + c_2 = 0$ to write

$$\begin{aligned} Q_3(\omega, \boldsymbol{A}) = 4 \sum_{j=0}^{2} c_j \bigg(\sum_{k=1}^{3} \frac{i\omega}{D_{m_0,0} + i\omega} \Big(\frac{1}{D_{m_0,0} + i\omega} \big(\boldsymbol{\alpha} \cdot A - V \big) \Big)^k \times \\ \times \Big(\frac{i\omega}{D_{m_j,0} + i\omega} - \frac{i\omega}{D_{m_0,0} + i\omega} \Big) \Big(\big(\boldsymbol{\alpha} \cdot A - V \big) \frac{1}{D_{m_j,0} + i\omega} \Big)^{3-k} \\ + \Big(\frac{i\omega}{(D_{m_j,0} + i\omega)^2} - \frac{i\omega}{(D_{m_0,0} + i\omega)^2} \Big) \Big(\big(\boldsymbol{\alpha} \cdot A - V \big) \frac{1}{D_{m_j,0} + i\omega} \Big)^3. \end{aligned}$$

Using inequality (3.16), we deduce that

$$\big\|Q_3(\omega,\boldsymbol{A})\big\|_{\mathfrak{S}_1} \leq K\bigg(\sum_{j=0}^{2}|c_j|(m_j-m_0)\bigg)\frac{|\omega|}{(m_0^2+\omega^2)^{\frac{3}{2}}}\,\big\|\boldsymbol{A}\big\|_{L^3}^3,$$

which provides estimate (6.7) with

$$K_3 := \sum_{j=0}^{2}|c_j|\frac{m_j-m_0}{m_0}.$$

Inequalities (6.8) follow similarly. Applying the Sobolev inequality (3.12) to (6.8), we deduce that the integrals

$$\mathcal{Q}_n(\boldsymbol{A}) := \frac{1}{4\pi}\int_{\mathbb{R}}\big(Q_n(\omega,\boldsymbol{A})+Q_n(-\omega,\boldsymbol{A})\big)\,d\omega,$$

define locally trace-class operators on $L^2(\mathbb{R}^3,\mathbb{R}^4)$ for $3\leq n\leq 5$, as soon as $\boldsymbol{A}\in\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$. The related densities $\rho_n(\boldsymbol{A})$ and currents $j_n(\boldsymbol{A})$ are well-defined and locally integrable on $\mathbb{R}^3$. When $\boldsymbol{A}$ is moreover in $L^n(\mathbb{R}^3)$, inequality (6.7) guarantees that the operators $\mathcal{Q}_n(\boldsymbol{A})$ are trace-class, while the functions $\rho_n(\boldsymbol{A})$ and $j_n(\boldsymbol{A})$ are integrable on $\mathbb{R}^3$. The continuity in these spaces follows from multi-linearity.

For $n=1$, we refine our estimates using the cancellations provided by conditions (2.7). Following the lines of the analysis of the operator $R_1(\omega,\boldsymbol{A})$, we start by writing

$$Q_1(\omega,\boldsymbol{A})+Q_1(-\omega,\boldsymbol{A}) = Q_{1,1}(\omega,\boldsymbol{A})-Q_{1,2}(\omega,\boldsymbol{A}), \tag{6.9}$$

where

$$Q_{1,1}(\omega,\boldsymbol{A}) := 8\sum_{j=0}^{2}c_j\,\omega^2\frac{D_{m_j,0}}{(D_{m_j,0}^2+\omega^2)^2}\big\{\boldsymbol{\alpha}\cdot A-V,D_{m_j,0}\big\}_{\mathbb{R}^3}\frac{1}{D_{m_j,0}^2+\omega^2}, \tag{6.10}$$

and

$$Q_{1,2}(\omega,\boldsymbol{A}) := 4\sum_{j=0}^{2}c_j\,\omega^2\frac{1}{D_{m_j,0}^2+\omega^2}\big(\boldsymbol{\alpha}\cdot A-V\big)\frac{1}{D_{m_j,0}^2+\omega^2}.$$

As for the operator $Q_{1,2}(\omega,\boldsymbol{A})$, we combine conditions (2.7) with identities (3.26) to estimate

$$\big\|Q_{1,2}(\omega,\boldsymbol{A})\big\|_{\mathfrak{S}_1}\leq K\bigg(\sum_{j=0}^{2}|c_j|\big(m_j^2-m_0^2\big)^2\bigg)\frac{\omega^2}{(m_0^2+\omega^2)^{\frac{5}{2}}}\,\big\|\boldsymbol{A}\big\|_{L^1}. \tag{6.11}$$

In order to estimate the operator $Q_{1,1}(\omega,\boldsymbol{A})$, we eliminate the odd powers of the masses m_j in the numerator of the right-hand side of (6.10) by taking the $\mathbb{C}^4$–trace. Recall that

$$\big\{\boldsymbol{\alpha}\cdot A-V,D_{m_j,0}\big\}_{\mathbb{R}^3} = \big\{p,A-V\boldsymbol{\alpha}\big\}_{\mathbb{R}^3}+B\cdot\boldsymbol{\Sigma}-2m_jV\boldsymbol{\beta}.$$

Since

$$\mathrm{tr}_{\mathbb{C}^4}\left(\boldsymbol{\beta}^d\prod_{k=1}^{3}\boldsymbol{\alpha}_k^{d_k}\right)=0, \tag{6.12}$$

when d is odd, we obtain

$$\begin{aligned}\mathrm{tr}_{\mathbb{C}^4}\left(\mathfrak{m}\,Q_{1,1}(\omega,\boldsymbol{A})\right) := 8\sum_{j=0}^{2} c_j\,\omega^2\frac{1}{(D_{m_j,0}^2+\omega^2)^2}\bigg(-2m_j^2V\,\mathrm{tr}_{\mathbb{C}^4}\left(\mathfrak{m}\right)\\ +\mathrm{tr}_{\mathbb{C}^4}\left(\mathfrak{m}\big(\boldsymbol{\alpha}\cdot p\big)\big(\{p,A-V\boldsymbol{\alpha}\}_{\mathbb{R}^3}+B\cdot\boldsymbol{\Sigma}\big)\right)\bigg)\frac{1}{D_{m_j,0}^2+\omega^2},\end{aligned}$$

for any of the matrices $\mathfrak{m} = I_4, \boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \boldsymbol{\alpha}_3$. On the other hand, we can compute

$$\begin{aligned}\frac{1}{(p^2+m_j^2+\omega^2)^2} = \frac{1}{(p^2+m_0^2+\omega^2)^2}+\frac{m_0^2-m_j^2}{(p^2+m_j^2+\omega^2)(p^2+m_0^2+\omega^2)^2}\\ +\frac{m_0^2-m_j^2}{(p^2+m_j^2+\omega^2)^2(p^2+m_0^2+\omega^2)},\end{aligned}\tag{6.13}$$

as well as

$$\begin{aligned}\frac{1}{(p^2+m_j^2+\omega^2)^2} = \frac{1}{(p^2+m_0^2+\omega^2)^2}+\frac{2(m_0^2-m_j^2)}{(p^2+m_0^2+\omega^2)^3}\\ +\frac{2(m_0^2-m_j^2)^2}{(p^2+m_j^2+\omega^2)(p^2+m_0^2+\omega^2)^3}+\frac{(m_0^2-m_j^2)^2}{(p^2+m_j^2+\omega^2)^2(p^2+m_0^2+\omega^2)^2}.\end{aligned}$$

Combining again with conditions (2.7) and identities (3.26), we obtain the estimate

$$\begin{aligned}\left\|\,\mathrm{tr}_{\mathbb{C}^4}\left(\mathfrak{m}\,Q_{1,1}(\omega,\boldsymbol{A})\right)\right\|_{\mathfrak{S}_1} \leq K\sum_{j=0}^{2}|c_j|\big(m_j^2-m_0^2\big)\,\frac{\omega^2}{(m_0^2+\omega^2)^{\frac{5}{2}}}\times\\ \times\Big(m_j^2\big\|V\big\|_{L^1}+\big(m_j^2-m_0^2\big)\big\|\boldsymbol{A}\big\|_{L^1}\Big).\end{aligned}$$

In view of (6.9) and (6.11), we have

$$\begin{aligned}\int_{\mathbb{R}}\left\|\,\mathrm{tr}_{\mathbb{C}^4}\left(\mathfrak{m}\left(Q_1(\omega,\boldsymbol{A})+Q_1(-\omega,\boldsymbol{A})\right)\right)\right\|_{\mathfrak{S}_1}d\omega\\ \leq K\sum_{j=0}^{2}|c_j|\left(m_j^2-m_0^2\right)\left(\frac{m_j^2}{m_0^2}\left\|V\right\|_{L^1}+\frac{m_j^2-m_0^2}{m_0^2}\left\|\boldsymbol{A}\right\|_{L^1}\right).\end{aligned}\tag{6.14}$$

Similarly, we can check that

$$\begin{aligned}\int_{\mathbb{R}}\left\|\,\mathrm{tr}_{\mathbb{C}^4}\left(\mathfrak{m}\,\chi\big(Q_1(\omega,\boldsymbol{A})+Q_1(-\omega,\boldsymbol{A})\big)\chi\right)\right\|_{\mathfrak{S}_1}d\omega\\ \leq K\sum_{j=0}^{2}|c_j|\left(m_j^2-m_0^2\right)\left(\frac{m_j^2}{m_0^2}\left\|V\right\|_{L^6}+\frac{m_j^2-m_0^2}{m_0^2}\left\|\boldsymbol{A}\right\|_{L^6}\right)\left\|\chi\right\|_{L^{\frac{12}{5}}}^2.\end{aligned}\tag{6.15}$$

For $n = 2$, the analysis is identical. We compute

$$Q_2(\omega,\boldsymbol{A})+Q_2(-\omega,\boldsymbol{A}) = Q_{2,1}(\omega,\boldsymbol{A})-Q_{2,2}(\omega,\boldsymbol{A}),\tag{6.16}$$

where

$$Q_{2,1}(\omega, \boldsymbol{A}) := 12 \sum_{j=0}^{2} c_j \, \omega^2 \times$$
$$\times \Big(\frac{D_{m_j,0}}{(D_{m_j,0}^2 + \omega^2)^2} \big\{ \boldsymbol{\alpha} \cdot A - V, D_{m_j,0} \big\} \frac{1}{D_{m_j,0}^2 + \omega^2} (\boldsymbol{\alpha} \cdot A - V) \frac{D_{m_j,0}}{D_{m_j,0}^2 + \omega^2}$$
$$+ \frac{D_{m_j,0}^2}{(D_{m_j,0}^2 + \omega^2)^2} \big\{ \boldsymbol{\alpha} \cdot A - V, D_{m_j,0} \big\} \frac{1}{D_{m_j,0}^2 + \omega^2} (\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0}^2 + \omega^2} \Big),$$

and

$$Q_{2,2}(\omega, \boldsymbol{A}) := 6 \sum_{j=0}^{2} c_j \, \omega^2 \Big(\frac{2 D_{m_j,0}}{D_{m_j,0}^2 + \omega^2} \Big((\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0}^2 + \omega^2} \Big)^2$$
$$+ \frac{1}{D_{m_j,0}^2 + \omega^2} (\boldsymbol{\alpha} \cdot A - V) \frac{D_{m_j,0}}{D_{m_j,0}^2 + \omega^2} (\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0}^2 + \omega^2}$$
$$+ \Big(\frac{1}{D_{m_j,0}^2 + \omega^2} (\boldsymbol{\alpha} \cdot A - V) \Big)^2 \frac{D_{m_j,0}}{D_{m_j,0}^2 + \omega^2} \Big).$$

In order to estimate the operators $Q_{2,1}(\omega, \boldsymbol{A})$ and $Q_{2,2}(\omega, \boldsymbol{A})$, we again take the $\mathbb{C}^4$–trace. For $\mathfrak{m} = I_4$ or $\mathfrak{m} = \boldsymbol{\alpha}_k$, we derive from (6.12) that

$$\mathrm{tr}_{\mathbb{C}^4} \big(\mathfrak{m} \, Q_{2,1}(\omega, \boldsymbol{A}) \big) = 12 \sum_{j=0}^{2} c_j \, \omega^2 \times$$
$$\times \, \mathrm{tr}_{\mathbb{C}^4} \Big(\frac{\mathfrak{m} (\boldsymbol{\alpha} \cdot p)}{(D_{m_j,0}^2 + \omega^2)^2} \big\{ \boldsymbol{\alpha} \cdot A - V, \boldsymbol{\alpha} \cdot p \big\} \frac{1}{D_{m_j,0}^2 + \omega^2} (\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0}^2 + \omega^2}$$
$$- m_j^2 \, \mathfrak{m} \frac{1}{(D_{m_j,0}^2 + \omega^2)^2} \big\{ \boldsymbol{\alpha} \cdot A + V, \boldsymbol{\alpha} \cdot p \big\} \frac{1}{D_{m_j,0}^2 + \omega^2} (\boldsymbol{\alpha} \cdot A + V) \frac{1}{D_{m_j,0}^2 + \omega^2}$$
$$- 2 m_j^2 \, \mathfrak{m} \frac{1}{(D_{m_j,0}^2 + \omega^2)^2} V \frac{1}{D_{m_j,0}^2 + \omega^2} (\boldsymbol{\alpha} \cdot A - V) \frac{\boldsymbol{\alpha} \cdot p}{D_{m_j,0}^2 + \omega^2}$$
$$+ 2 m_j^2 \, \mathfrak{m} \frac{\boldsymbol{\alpha} \cdot p}{(D_{m_j,0}^2 + \omega^2)^2} V \frac{1}{D_{m_j,0}^2 + \omega^2} (\boldsymbol{\alpha} \cdot A + V) \frac{1}{D_{m_j,0}^2 + \omega^2}$$
$$+ \mathfrak{m} \frac{p^2 + m_j^2}{(D_{m_j,0}^2 + \omega^2)^2} \big\{ \boldsymbol{\alpha} \cdot A - V, \boldsymbol{\alpha} \cdot p \big\} \frac{1}{D_{m_j,0}^2 + \omega^2} (\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0}^2 + \omega^2} \Big),$$

while

$$\mathrm{tr}_{\mathbb{C}^4} \big(\mathfrak{m} \, Q_{2,2}(\omega, \boldsymbol{A}) \big) = 6 \sum_{j=0}^{2} c_j \, \omega^2 \, \mathrm{tr}_{\mathbb{C}^4} \Big(2 \mathfrak{m} \frac{\boldsymbol{\alpha} \cdot p}{D_{m_j,0}^2 + \omega^2} \times$$
$$\times \Big((\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0}^2 + \omega^2} \Big)^2 + \mathfrak{m} \frac{1}{D_{m_j,0}^2 + \omega^2} (\boldsymbol{\alpha} \cdot A - V) \frac{\boldsymbol{\alpha} \cdot p}{D_{m_j,0}^2 + \omega^2} \times$$
$$\times (\boldsymbol{\alpha} \cdot A - V) \frac{1}{D_{m_j,0}^2 + \omega^2} + \mathfrak{m} \Big(\frac{1}{D_{m_j,0}^2 + \omega^2} (\boldsymbol{\alpha} \cdot A - V) \Big)^2 \frac{\boldsymbol{\alpha} \cdot p}{D_{m_j,0}^2 + \omega^2} \Big).$$

Invoking conditions (2.7), as well as identities (3.26) and (6.13), we deduce that

$$\left\| \mathrm{tr}_{\mathbb{C}^4} \left(\mathfrak{m}\, Q_{2,1}(\omega, \boldsymbol{A}) \right) \right\|_{\mathfrak{S}_1} \leq K \sum_{j=0}^{2} |c_j| \left(\left(m_j^2 - m_0^2 \right) \left\| \boldsymbol{A} \right\|_{L^2}^2 \frac{\omega^2}{(m_0^2+\omega^2)^2} + m_j^2 \left\| \boldsymbol{A} \right\|_{L^2} \left(\left\| \boldsymbol{A} \right\|_{L^2} + \left\| V \right\|_{L^2} \right) \frac{\omega^2}{(m_j^2+\omega^2)^2} \right),$$

and

$$\left\| \mathrm{tr}_{\mathbb{C}^4} \left(\mathfrak{m}\, Q_{2,2}(\omega, \boldsymbol{A}) \right) \right\|_{\mathfrak{S}_1} \leq K \left(\sum_{j=0}^{2} |c_j| \left(m_j^2 - m_0^2 \right) \right) \left\| \boldsymbol{A} \right\|_{L^2}^2 \frac{\omega^2}{(m_0^2+\omega^2)^2}.$$

It follows that

$$\begin{aligned} &\int_{\mathbb{R}} \left\| \mathrm{tr}_{\mathbb{C}^4} \left(\mathfrak{m} \left(Q_2(\omega, \boldsymbol{A}) + Q_2(-\omega, \boldsymbol{A}) \right) \right) \right\|_{\mathfrak{S}_1} d\omega \\ &\quad \leq K \sum_{j=0}^{2} |c_j| \left(\frac{m_j^2 - m_0^2}{m_0} \left\| \boldsymbol{A} \right\|_{L^2}^2 + m_j \left\| \boldsymbol{A} \right\|_{L^2} \left(\left\| \boldsymbol{A} \right\|_{L^2} + \left\| V \right\|_{L^2} \right) \right). \end{aligned}$$

Similarly, we have

$$\begin{aligned} &\int_{\mathbb{R}} \left\| \mathrm{tr}_{\mathbb{C}^4} \left(\mathfrak{m}\, \chi \big(Q_2(\omega, \boldsymbol{A}) + Q_2(-\omega, \boldsymbol{A}) \big) \chi \right) \right\|_{\mathfrak{S}_1} d\omega \\ &\quad \leq K \sum_{j=0}^{2} |c_j| \left(\frac{m_j^2 - m_0^2}{m_0} \left\| \boldsymbol{A} \right\|_{L^6}^2 + m_j \left\| \boldsymbol{A} \right\|_{L^6} \left(\left\| \boldsymbol{A} \right\|_{L^6} + \left\| V \right\|_{L^6} \right) \right) \left\| \chi \right\|_{L^3}^2. \end{aligned} \tag{6.17}$$

In view of (6.14) and (6.15), we conclude that the integrals

$$\mathrm{tr}_{\mathbb{C}^4} \left(\mathfrak{m}\, \mathcal{Q}_n \right) := \frac{1}{4\pi} \int_{\mathbb{R}} \mathrm{tr}_{\mathbb{C}^4} \left(\mathfrak{m} \left(Q_n(\omega, \boldsymbol{A}) + Q_n(-\omega, \boldsymbol{A}) \right) \right) d\omega,$$

also define local trace-class operators on $L^2(\mathbb{R}^3, \mathbb{R}^4)$ for $n = 1, 2$, as soon as $\boldsymbol{A} \in \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$. The operators are trace-class when $\boldsymbol{A}$ is in $L^n(\mathbb{R}^3)$. Concerning the related densities $\rho_n(\boldsymbol{A})$ and currents $j_n(\boldsymbol{A})$, they are well-defined and locally integrable on $\mathbb{R}^3$ for $\boldsymbol{A} \in \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$, and integrable on $\mathbb{R}^3$ for $\boldsymbol{A} \in L^n(\mathbb{R}^3)$. Their continuity follows again by multi-linearity.

At this stage, it remains to recall Formulas (6.3) and (6.5) to complete the proof of Lemma 6.1. □

We are now in position to complete the proof of Theorem 2.2.

End of the proof of Theorem 2.2. We have shown that the functional $\mathcal{F}_{\mathrm{PV}}$ is smooth on the open subset $\mathcal{H}$ of four-potentials $\boldsymbol{A}$ such that 0 is not an eigenvalue of $D_{m_j, \boldsymbol{A}}$ for each $j = 0, 1, 2$. In particular, the differential $\mathrm{d}\mathcal{F}_{\mathrm{PV}}(\boldsymbol{A})$ is a bounded form on $\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$. By duality, it can be identified with a couple of functions (ρ_*, j_*) in the Coulomb space $\mathcal{C}$ defined in (2.21). Our task reduces to verify that $\rho_* = \rho_{\boldsymbol{A}}$ and $j_* = -j_{\boldsymbol{A}}$.

We first restrict our attention to four-potentials $\boldsymbol{A}$ which are moreover integrable on $\mathbb{R}^3$. In this case, the functional $\mathcal{F}_{\mathrm{PV}}(\boldsymbol{A})$ is given by Formula (2.12), which may be written in view of (4.1) as

$$\mathcal{F}_{\mathrm{PV}}(\boldsymbol{A}) = \sum_{n=1}^{5} \mathcal{F}_n(\boldsymbol{A}) + \mathcal{R}_6(\boldsymbol{A}),$$

where we recall that

$$\mathcal{F}_n(\boldsymbol{A}) := \frac{1}{4\pi} \int_{\mathbb{R}} \mathrm{tr}\, \Big(\mathrm{tr}_{\mathbb{C}^4} \big(R_n(\omega, \boldsymbol{A}) + R_n(-\omega, \boldsymbol{A}) \big) \Big)\, d\omega,$$

and

$$\mathcal{R}_6(\boldsymbol{A}) := \frac{1}{4\pi} \int_{\mathbb{R}} \mathrm{tr}\, \Big(\mathrm{tr}_{\mathbb{C}^4} \big(R'_6(\omega, \boldsymbol{A}) + R'_6(-\omega, \boldsymbol{A}) \big)\, d\omega.$$

We have computed the differential of $\mathrm{d}\mathcal{R}_6(\boldsymbol{A})$ in (4.56). On the other hand, the functionals $\mathcal{F}_n$ are n-linear with respect to $\boldsymbol{A}$, so that their differentials are given by

$$\begin{aligned} &\mathrm{d}\mathcal{F}_n(\boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) \\ &\quad = \frac{1}{4\pi} \int_{\mathbb{R}} \mathrm{tr}\, \Big(\mathrm{tr}_{\mathbb{C}^4} \big(\mathrm{d}_{\boldsymbol{A}} R_n(\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) + \mathrm{d}_{\boldsymbol{A}} R_n(-\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) \big) \Big)\, d\omega, \end{aligned}$$

with

$$\begin{aligned} \mathrm{d}_{\boldsymbol{A}} R_n(\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) = \sum_{j=0}^{2} c_j \, \frac{i\omega}{D_{m_j,0} + i\omega} \sum_{k=0}^{n-1} \Big(\big(\boldsymbol{\alpha} \cdot A - V \big) \frac{1}{D_{m_j,0} + i\omega} \Big)^k \times \\ \times \big(\boldsymbol{\alpha} \cdot \mathfrak{a} - \mathfrak{v} \big) \frac{1}{D_{m_j,0} + i\omega} \Big(\big(\boldsymbol{\alpha} \cdot A - V \big) \frac{1}{D_{m_j,0} + i\omega} \Big)^{n-1-k}, \end{aligned} \tag{6.18}$$

for any $(\mathfrak{v}, \mathfrak{a}) \in L^1(\mathbb{R}^3, \mathbb{R}^4) \cap \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$. It follows that the differential $\mathrm{d}\mathcal{F}_{\mathrm{PV}}(\boldsymbol{A})$ is equal to

$$\mathrm{d}\mathcal{F}_{\mathrm{PV}}(\boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) = \frac{1}{4\pi} \int_{\mathbb{R}} \Xi(\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a})\, d\omega,$$

with

$$\begin{aligned} \Xi(\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) := \mathrm{tr} \Bigg(\sum_{n=1}^{5} \mathrm{tr}\, \Big(\mathrm{tr}_{\mathbb{C}^4} \big(\mathrm{d}_{\boldsymbol{A}} R_n(\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) + \mathrm{d}_{\boldsymbol{A}} R_n(-\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) \big) \Big) \\ + \mathrm{tr}\, \Big(\mathrm{tr}_{\mathbb{C}^4} \big(\mathrm{d}_{\boldsymbol{A}} R'_6(\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) + \mathrm{d}_{\boldsymbol{A}} R'_6(-\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) \big) \Big) \Bigg). \end{aligned}$$

At this stage, we make use of Formulas (4.53) and (6.18) to check that

$$\Xi(\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a}) = \mathrm{tr} \left(\mathrm{tr}_{\mathbb{C}^4} \left(\sum_{j=0}^{2} c_j \, \frac{i\omega}{(D_{m_j,\boldsymbol{A}} + i\omega)^2} \big(\boldsymbol{\alpha} \cdot \mathfrak{a} - \mathfrak{v} \big) \right) \right). \tag{6.19}$$

Indeed, we have established in the course of Lemma 4.6 that each term in the decomposition of $\mathrm{d}_{\boldsymbol{A}} R'_6(\omega, \boldsymbol{A})(\mathfrak{v}, \mathfrak{a})$ which is provided by Formula (4.53)

is trace-class. As a consequence, we can write

$$\begin{aligned}
&\mathrm{tr}\Big(\mathrm{tr}_{\mathbb{C}^4}\ \mathrm{d}_{\boldsymbol{A}} R_6'(\omega,\boldsymbol{A})(\mathfrak{v},\mathfrak{a})\Big)\\
&\quad= \sum_{j=0}^{2} c_j\ \mathrm{tr}\ \frac{i\omega}{D_{m_j,\boldsymbol{A}}+i\omega}\big(\boldsymbol{\alpha}\cdot\mathfrak{a}-\mathfrak{v}\big)\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\Big(\big(\boldsymbol{\alpha}\cdot A-V\big)\frac{1}{D_{m_j,0}+i\omega}\Big)^6\\
&\quad+\sum_{j=0}^{2} c_j\ \sum_{k=0}^{5}\mathrm{tr}\ \frac{i\omega}{D_{m_j,\boldsymbol{A}}+i\omega}\Big(\big(\boldsymbol{\alpha}\cdot A-V\big)\frac{1}{D_{m_j,0}+i\omega}\Big)^{5-k}\times\\
&\qquad\times\big(\boldsymbol{\alpha}\cdot\mathfrak{a}-\mathfrak{v}\big)\frac{1}{D_{m_j,0}+i\omega}\Big(\big(\boldsymbol{\alpha}\cdot A-V\big)\frac{1}{D_{m_j,0}+i\omega}\Big)^{k}.
\end{aligned}$$

An advantage of this further decomposition is that we are allowed to commute the products in the right-hand side, so as to obtain

$$\begin{aligned}
&\mathrm{tr}\Big(\mathrm{tr}_{\mathbb{C}^4}\ \mathrm{d}_{\boldsymbol{A}} R_6'(\omega,\boldsymbol{A})(\mathfrak{v},\mathfrak{a})\Big)\\
&\quad= \sum_{j=0}^{2} c_j\ \mathrm{tr}\ \frac{i\omega}{D_{m_j,\boldsymbol{A}}+i\omega}\Big(\big(\boldsymbol{\alpha}\cdot A-V\big)\frac{1}{D_{m_j,0}+i\omega}\Big)^6\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\big(\boldsymbol{\alpha}\cdot\mathfrak{a}-\mathfrak{v}\big)\\
&\quad+\sum_{j=0}^{2} c_j\ \sum_{k=0}^{5}\mathrm{tr}\ \frac{i\omega}{D_{m_j,0}+i\omega}\Big(\big(\boldsymbol{\alpha}\cdot A-V\big)\frac{1}{D_{m_j,0}+i\omega}\Big)^{k}\frac{1}{D_{m_j,\boldsymbol{A}}+i\omega}\times\\
&\qquad\times\Big(\big(\boldsymbol{\alpha}\cdot A-V\big)\frac{1}{D_{m_j,0}+i\omega}\Big)^{5-k}\big(\boldsymbol{\alpha}\cdot\mathfrak{a}-\mathfrak{v}\big).
\end{aligned}$$

This follows from the property that the operator $(i\omega)(D_{m_j,\boldsymbol{A}}+i\omega)^{-1}$ is bounded, while the operators $(\boldsymbol{\alpha}\cdot A-V)(D_{m_j,0}+i\omega)^{-1}$ and $(\boldsymbol{\alpha}\cdot\mathfrak{a}-\mathfrak{v})(D_{m_j,0}+i\omega)^{-1}$ belong to suitable Schatten spaces. Using the resolvent expansion (3.6), we are led to

$$\begin{aligned}
\mathrm{tr}\Big(\mathrm{tr}_{\mathbb{C}^4}\,\mathrm{d}_{\boldsymbol{A}} R_6'(\omega,\boldsymbol{A})(\mathfrak{v},\mathfrak{a})\Big) &= \mathrm{tr}\Big(\mathrm{tr}_{\mathbb{C}^4}\sum_{j=0}^{2} c_j\Big(\frac{i\omega}{(D_{m_j,\boldsymbol{A}}+i\omega)^2}\big(\boldsymbol{\alpha}\cdot\mathfrak{a}-\mathfrak{v}\big)\\
&\quad-\sum_{k=0}^{4}\sum_{l=0}^{4-k}\frac{1}{D_{m_j,0}+i\omega}\Big(\big(\boldsymbol{\alpha}\cdot A-V\big)\frac{1}{D_{m_j,0}+i\omega}\Big)^{k}\frac{i\omega}{D_{m_j,0}+i\omega}\times\\
&\qquad\times\Big(\big(\boldsymbol{\alpha}\cdot A-V\big)\frac{1}{D_{m_j,0}+i\omega}\Big)^{l}\big(\boldsymbol{\alpha}\cdot\mathfrak{a}-\mathfrak{v}\big)\Big)\Big).
\end{aligned}\tag{6.20}$$

Similarly, we can deduce from (6.18) that

$$\begin{aligned}
&\mathrm{tr}\Big(\mathrm{tr}_{\mathbb{C}^4}\,\mathrm{d}_{\boldsymbol{A}} R_n(\omega,\boldsymbol{A})(\mathfrak{v},\mathfrak{a})\Big)\\
&\quad=\mathrm{tr}\Big(\mathrm{tr}_{\mathbb{C}^4}\sum_{j=0}^{2} c_j\ \sum_{k=0}^{n-1}\frac{1}{D_{m_j,0}+i\omega}\Big(\big(\boldsymbol{\alpha}\cdot A-V\big)\frac{1}{D_{m_j,0}+i\omega}\Big)^{n-1-k}\times\\
&\qquad\times\frac{i\omega}{D_{m_j,0}+i\omega}\Big(\big(\boldsymbol{\alpha}\cdot A-V\big)\frac{1}{D_{m_j,0}+i\omega}\Big)^{k}\big(\boldsymbol{\alpha}\cdot\mathfrak{a}-\mathfrak{v}\big)\Big).
\end{aligned}$$

Formula (6.19) follows combining with (6.20).

As a conclusion, we have derived the following expression of $\mathrm{d}\mathcal{F}_{\mathrm{PV}}(\boldsymbol{A})$,

$$\mathrm{d}\mathcal{F}_{\mathrm{PV}}(\boldsymbol{A})(\mathfrak{v},\mathfrak{a}) = \frac{1}{4\pi}\int_{\mathbb{R}} \mathrm{tr}\,\Big(\mathrm{tr}_{\mathbb{C}^4}\Big(\sum_{j=0}^{2} c_j \Big(\frac{i\omega}{(D_{m_j,\boldsymbol{A}}+i\omega)^2} - \frac{i\omega}{(D_{m_j,\boldsymbol{A}}-i\omega)^2}\Big)\big(\boldsymbol{\alpha}\cdot\mathfrak{a}-\mathfrak{v}\big)\,d\omega\Big)\Big).$$

In view of (6.1) and Lemma 6.1, we deduce that

$$\mathrm{d}\mathcal{F}_{\mathrm{PV}}(\boldsymbol{A})(\mathfrak{v},\mathfrak{a}) = \mathrm{tr}\,\Big(\mathrm{tr}_{\mathbb{C}^4}\Big(Q_{\boldsymbol{A}}\big(\mathfrak{v}-\boldsymbol{\alpha}\cdot\mathfrak{a}\big)\Big)\Big) = \int_{\mathbb{R}^3}\big(\rho_{\boldsymbol{A}}\mathfrak{v} - j_{\boldsymbol{A}}\cdot\mathfrak{a}\big),$$

so that $\rho_* = \rho_{\boldsymbol{A}}$ and $j_* = j_{\boldsymbol{A}}$, when $\boldsymbol{A}\in L^1(\mathbb{R}^3,\mathbb{R}^4)\cap \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$.

In the general case where $\boldsymbol{A}$ is only in $\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$, we can construct a sequence of maps $(\boldsymbol{A}_n)_{n\in\mathbb{N}}$ in $L^1(\mathbb{R}^3,\mathbb{R}^4)\cap\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$, for which $0\notin\sigma(D_{m_j,\boldsymbol{A}_n})$ for any $n\in\mathbb{N}$ and each $j=0,1,2$, and such that

$$\boldsymbol{A}_n \to \boldsymbol{A} \quad \text{in} \quad \dot{H}^1_{\mathrm{div}}(\mathbb{R}^3),$$

as $n\to\infty$. The existence of such a sequence follows from the density of $L^1(\mathbb{R}^3,\mathbb{R}^4)\cap\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$ in $\dot{H}^1_{\mathrm{div}}(\mathbb{R}^3)$, and statement (ii) in Lemma 2.1. For each integer n, we know that

$$\mathrm{d}\mathcal{F}_{\mathrm{PV}}(\boldsymbol{A}_n)(\mathfrak{v},\mathfrak{a}) = \int_{\mathbb{R}^3}\Big(\rho_{\boldsymbol{A}_n}\mathfrak{v} - j_{\boldsymbol{A}_n}\cdot\mathfrak{a}\Big),$$

for any four-potential $(\mathfrak{v},\mathfrak{a})\in\mathcal{C}^\infty_c(\mathbb{R}^3,\mathbb{R}^4)$. Combining the continuous differentiability of the functional $\mathcal{F}_{\mathrm{PV}}$ with statement (i) in Lemma 6.1, we obtain, taking the limit $n\to\infty$,

$$\mathrm{d}\mathcal{F}_{\mathrm{PV}}(\boldsymbol{A})(\mathfrak{v},\mathfrak{a}) = \int_{\mathbb{R}^3}\Big(\rho_{\boldsymbol{A}}\mathfrak{v} - j_{\boldsymbol{A}}\cdot\mathfrak{a}\Big),$$

which completes the proof of (ii) in Theorem 2.2.

Concerning (iii), recall that the second order differential of $\mathcal{F}_{\mathrm{PV}}$ is equal to

$$\mathrm{d}^2\mathcal{F}_{\mathrm{PV}}(\boldsymbol{A}) = \mathrm{d}^2\mathcal{F}_2(\boldsymbol{F}) + \mathrm{d}^2\mathcal{F}_4(\boldsymbol{A}) + \mathrm{d}^2\mathcal{R}(\boldsymbol{A}).$$

Since $\mathcal{F}_2$ is quadratic and $\mathcal{F}_4$ is quartic, estimate (2.22) appears as a consequence of Formula (2.15), and inequalities (4.19) and (4.57). This completes the proof of Theorem 2.2. □

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