

ON HIGHER ORDER ESTIMATES
IN QUANTUM ELECTRODYNAMICS

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ABSTRACT. We propose a new method to derive certain higher order estimates in quantum electrodynamics. Our method is particularly convenient in the application to the non-local semi-relativistic models of quantum electrodynamics as it avoids the use of iterated commutator expansions. We re-derive higher order estimates obtained earlier by Fröhlich, Griesemer, and Schlein and prove new estimates for a non-local molecular no-pair operator.

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1. INTRODUCTION

The main objective of this paper is to present a new method to derive higher order estimates in quantum electrodynamics (QED) of the form

$$(1.1) \quad \| H_f^{n/2} (H + C)^{-n/2} \| \leq \text{const} < \infty,$$

$$(1.2) \quad \| [H_f^{n/2}, H] (H + C)^{-n/2} \| \leq \text{const} < \infty,$$

for all $n \in \mathbb{N}$, where $C > 0$ is sufficiently large. In these bounds H_f denotes the radiation field energy of the quantized photon field and H is the full Hamiltonian generating the time evolution of an interacting electron-photon system. For instance, estimates of this type serve as one of the main technical ingredients in the mathematical analysis of Rayleigh scattering. In this context, (1.1) has been proven by Fröhlich et al. in the case where H is the non- or semi-relativistic Pauli-Fierz Hamiltonian [4]; a slightly weaker version of (1.2) has been obtained in [4] for all even values of n . Higher order estimates of the form (1.1) also turn out to be useful in the study of the existence of ground states in a no-pair model of QED [8]. In fact, they imply that every eigenvector of the Hamiltonian H or spectral subspaces of H corresponding to some bounded interval are contained in the domains of higher powers of H_f . This information

is very helpful in order to overcome numerous technical difficulties which are caused by the non-locality of the no-pair operator. In these applications it is actually necessary to have some control on the norms in (1.1) and (1.2) when the operator H gets modified. To this end we shall give rough bounds on the right hand sides of (1.1) and (1.2) in terms of the ground state energy and integrals involving the form factor and the dispersion relation.

Various types of higher order estimates have actually been employed in the mathematical analysis of quantum field theories since a very long time. Here we only mention the classical works [5, 11] on $P(\phi)_2$ models and the more recent articles [2] again on a $P(\phi)_2$ model and [1] on the Nelson model.

In what follows we briefly describe the organization and the content of the present article. In Section 2 we develop the main idea behind our techniques in a general setting. By the criterion established there the proof of the higher order estimates is essentially boiled down to the verification of certain form bounds on the commutator between H and a regularized version of $H_f^{n/2}$. After that, in Section 3, we introduce some of the most important operators appearing in QED and establish some useful norm bounds on certain commutators involving them. These commutator estimates provide the main ingredients necessary to apply the general criterion of Section 2 to the QED models treated in this article. Their derivation is essentially based on the pull-through formula which is always employed either way to derive higher order estimates in quantum field theories [1, 2, 4, 5, 11]; compare Lemma 3.2 below. In Sections 4, 5, and 6 the general strategy from Section 2 is applied to the non- and semi-relativistic Pauli-Fierz operators and to the no-pair operator, respectively. The latter operators are introduced in detail in these sections. Apart from the fact that our estimate (1.2) is slightly stronger than the corresponding one of [4] the results of Sections 4 and 5 are not new and have been obtained earlier in [4]. However, in order to prove the higher order estimate (1.1) for the no-pair operator we virtually have to re-derive it for the semi-relativistic Pauli-Fierz operator by our own method anyway. Moreover, we think that the arguments employed in Sections 4 and 5 are more convenient and less involved than the procedure carried through in [4]. The main text is followed by an appendix where we show that the semi-relativistic Pauli-Fierz operator for a molecular system with static nuclei is semi-bounded below, provided that all Coulomb coupling constants are less than or equal to $2/\pi$. Moreover, we prove the same result for a molecular no-pair operator assuming that all Coulomb coupling constants are strictly less than the critical coupling constant of the Brown-Ravenhall model [3]. The results of the appendix are based on corresponding estimates for hydrogen-like atoms obtained in [10]. (We remark that the considerably stronger stability of matter of the second kind has been proven for a molecular no-pair operator in [9] under more restrictive assumptions on the involved physical parameters.) No restrictions on the values of the fine-structure constant or on the ultra-violet cut-off are imposed in the present article.

The main new results of this paper are Theorem 2.1 and its corollaries which provide general criteria for the validity of higher order estimates and Theorem 6.1 where higher order estimates for the no-pair operator are established.

Some frequently used notation. For $a, b \in \mathbb{R}$, we write $a \wedge b := \min\{a, b\}$ and $a \vee b := \max\{a, b\}$. $\mathcal{D}(T)$ denotes the domain of some operator T acting in some Hilbert space and $\mathcal{Q}(T)$ its form domain, when T is semi-bounded below. $C(a, b, \dots), C'(a, b, \dots)$, etc. denote constants that depend only on the quantities a, b, \dots and whose value might change from one estimate to another.

2. HIGHER ORDER ESTIMATES: A GENERAL CRITERION

The following theorem and its succeeding corollaries present the key idea behind of our method. They essentially reduce the derivation of the higher order estimates to the verification of a certain sequence of form bounds. These form bounds can be verified easily without any further induction argument in the QED models treated in this paper.

THEOREM 2.1. *Let H and F_ε , $\varepsilon > 0$, be self-adjoint operators in some Hilbert space \mathcal{H} such that $H \geq 1$, $F_\varepsilon \geq 0$, and each F_ε is bounded. Let $m \in \mathbb{N} \cup \{\infty\}$, let \mathcal{D} be a form core for H , and assume that the following conditions are fulfilled:*

- (a) *For every $\varepsilon > 0$, F_ε maps \mathcal{D} into $\mathcal{Q}(H)$ and there is some $c_\varepsilon \in (0, \infty)$ such that*

$$\langle F_\varepsilon \psi | H F_\varepsilon \psi \rangle \leq c_\varepsilon \langle \psi | H \psi \rangle, \quad \psi \in \mathcal{D}.$$

- (b) *There is some $c \in [1, \infty)$ such that, for all $\varepsilon > 0$,*

$$\langle \psi | F_\varepsilon^2 \psi \rangle \leq c^2 \langle \psi | H \psi \rangle, \quad \psi \in \mathcal{D}.$$

- (c) *For every $n \in \mathbb{N}$, $n < m$, there is some $c_n \in [1, \infty)$ such that, for all $\varepsilon > 0$,*

$$\begin{aligned} & \left| \langle H \varphi_1 | F_\varepsilon^n \varphi_2 \rangle - \langle F_\varepsilon^n \varphi_1 | H \varphi_2 \rangle \right| \\ & \leq c_n \left\{ \langle \varphi_1 | H \varphi_1 \rangle + \langle F_\varepsilon^{n-1} \varphi_2 | H F_\varepsilon^{n-1} \varphi_2 \rangle \right\}, \quad \varphi_1, \varphi_2 \in \mathcal{D}. \end{aligned}$$

Then it follows that, for every $n \in \mathbb{N}$, $n < m + 1$,

$$(2.1) \quad \| F_\varepsilon^n H^{-n/2} \| \leq C_n := 4^{n-1} c^n \prod_{\ell=1}^{n-1} c_\ell.$$

(An empty product equals 1 by definition.)

Proof. We define

$$T_\varepsilon(n) := H^{1/2} [F_\varepsilon^{n-1}, H^{-1}] H^{-(n-2)/2}, \quad n \in \{2, 3, 4, \dots\}.$$

$T_\varepsilon(n)$ is well-defined and bounded because of the closed graph theorem and Condition (a), which implies that $F_\varepsilon \in \mathcal{L}(\mathcal{Q}(H))$, where $\mathcal{Q}(H) = \mathcal{D}(H^{1/2})$

is equipped with the form norm. We shall prove the following sequence of assertions by induction on $n \in \mathbb{N}$, $n < m + 1$.

$$(2.2) \quad A(n) \text{ :} \Leftrightarrow \quad \text{The bound (2.1) holds true and, if } n > 3, \text{ we have} \\ \forall \varepsilon > 0 : \quad \|T_\varepsilon(n)\| \leq C_n/4c^2.$$

For $n = 1$, the bound (2.1) is fulfilled with $C_1 = c$ on account of Condition (b). Next, assume that $n \in \mathbb{N}$, $n < m$, and that $A(1), \dots, A(n)$ hold true. To find a bound on $\|F_\varepsilon^{n+1} H^{-(n+1)/2}\|$ we write

$$(2.3) \quad F_\varepsilon^{n+1} H^{-(n+1)/2} = Q_1 + Q_2$$

with

$$Q_1 := F_\varepsilon H^{-1} F_\varepsilon^n H^{-(n-1)/2}, \quad Q_2 := F_\varepsilon [F_\varepsilon^n, H^{-1}] H^{-(n-1)/2}.$$

By the induction hypothesis we have

$$(2.4) \quad \|Q_1\| \leq \|F_\varepsilon H^{-1/2}\| \|H^{-1/2} F_\varepsilon\| \|F_\varepsilon^{n-1} H^{-(n-1)/2}\| \leq c^2 C_{n-1},$$

where $C_0 := 1$. Moreover, we observe that

$$(2.5) \quad \|Q_2\| = \|F_\varepsilon H^{-1/2} T_\varepsilon(n+1)\| \leq c \|T_\varepsilon(n+1)\|.$$

To find a bound on $\|T_\varepsilon(n+1)\|$ we recall that F_ε maps the form domain of H continuously into itself. In particular, since \mathcal{D} is a form core for H the form bound appearing in Condition (c) is available, for all $\varphi_1, \varphi_2 \in \mathcal{Q}(H)$. Let $\phi, \psi \in \mathcal{D}$. Applying Condition (c), extended in this way, with

$$\varphi_1 = \delta^{1/2} H^{-1/2} \phi \in \mathcal{Q}(H), \quad \varphi_2 = \delta^{-1/2} H^{-(n+1)/2} \psi \in \mathcal{Q}(H),$$

for some $\delta > 0$, we obtain

$$\begin{aligned} & |\langle \phi | T_\varepsilon(n+1) \psi \rangle| \\ &= |\langle H H^{-1/2} \phi | F_\varepsilon^n H^{-(n+1)/2} \psi \rangle - \langle F_\varepsilon^n H^{-1/2} \phi | H H^{-(n+1)/2} \psi \rangle| \\ &\leq c_n \inf_{\delta > 0} \{ \delta \|\phi\|^2 + \delta^{-1} \|\{H^{1/2} F_\varepsilon^{n-1} H^{-n/2}\} H^{-1/2} \psi\|^2 \} \\ &\leq 2c_n \|\{H^{1/2} F_\varepsilon^{n-1} H^{-n/2}\}\| \|\phi\| \|\psi\|. \end{aligned}$$

The operator $\{\dots\}$ is just the identity when $n = 1$. For $n > 1$, it can be written as

$$(2.6) \quad H^{1/2} F_\varepsilon^{n-1} H^{-n/2} = \{H^{-1/2} F_\varepsilon\} F_\varepsilon^{n-2} H^{-(n-2)/2} + T_\varepsilon(n).$$

Applying the induction hypothesis and $c, c_\ell \geq 1$, we thus get $\|T_\varepsilon(2)\| \leq 2c_1$, $\|T_\varepsilon(3)\| \leq 6cc_1c_2$, $\|T_\varepsilon(4)\| \leq 14c^2c_1c_2c_3 < C_4/4c^2$, and

$$\begin{aligned} c \|T_\varepsilon(n+1)\| &= c \sup \{ |\langle \phi | T_\varepsilon(n+1) \psi \rangle| : \phi, \psi \in \mathcal{D}, \|\phi\| = \|\psi\| = 1 \} \\ &\leq 2c_n (c^2 C_{n-2} + C_n/4c) < c_n C_n = C_{n+1}/4c, \quad n > 3, \end{aligned}$$

since $c^2 C_{n-2} \leq C_n/16$, for $n > 3$. Taking (2.3)–(2.5) into account we arrive at $\|F_\varepsilon^2 H^{-1}\| \leq c^2 + 2cc_1 < C_2$, $\|F_\varepsilon^3 H^{-3/2}\| \leq c^3 + 6c^2c_1c_2 < C_3$, and

$$\|F_\varepsilon^{n+1} H^{-(n+1)/2}\| < c^2 C_{n-2} + C_{n+1}/4c < C_{n+1}, \quad n > 3,$$

which concludes the induction step. \square

COROLLARY 2.2. Assume that H and F_ε , $\varepsilon > 0$, are self-adjoint operators in some Hilbert space \mathcal{H} that fulfill the assumptions of Theorem 2.1 with (c) replaced by the stronger condition

(c') For every $n \in \mathbb{N}$, $n < m$, there is some $c_n \in [1, \infty)$ such that, for all $\varepsilon > 0$,

$$\begin{aligned} & \left| \langle H \varphi_1 | F_\varepsilon^n \varphi_2 \rangle - \langle F_\varepsilon^n \varphi_1 | H \varphi_2 \rangle \right| \\ & \leq c_n \left\{ \|\varphi_1\|^2 + \langle F_\varepsilon^{n-1} \varphi_2 | H F_\varepsilon^{n-1} \varphi_2 \rangle \right\}, \quad \varphi_1, \varphi_2 \in \mathcal{D}. \end{aligned}$$

Then, in addition to (2.1), it follows that, for $n \in \mathbb{N}$, $n < m$, $[F_\varepsilon^n, H] H^{-n/2}$ defines a bounded sesquilinear form with domain $\mathcal{Q}(H) \times \mathcal{Q}(H)$ and

$$(2.7) \quad \|[F_\varepsilon^n, H] H^{-n/2}\| \leq C'_n := 4^n c^{n-1} \prod_{\ell=1}^n c_\ell.$$

Proof. Again, the form bound in (c') is available, for all $\varphi_1, \varphi_2 \in \mathcal{Q}(H)$, whence

$$\begin{aligned} & \left| \langle H \phi | F_\varepsilon^n H^{-n/2} \psi \rangle - \langle F_\varepsilon^n \phi | H H^{-n/2} \psi \rangle \right| \\ & \leq c_n \inf_{\delta > 0} \left\{ \delta \|\phi\|^2 + \delta^{-1} \|H^{1/2} F_\varepsilon^{n-1} H^{-n/2} \psi\|^2 \right\} \leq 2 c_n \|H^{1/2} F_\varepsilon^{n-1} H^{-n/2}\|, \end{aligned}$$

for all normalized $\phi, \psi \in \mathcal{Q}(H)$. The assertion now follows from (2.1), (2.6), and the bounds on $\|T_\varepsilon(n)\|$ given in the proof of Theorem 2.1. \square

COROLLARY 2.3. Let $H \geq 1$ and $A \geq 0$ be two self-adjoint operators in some Hilbert space \mathcal{H} . Let $\kappa > 0$, define

$$f_\varepsilon(t) := t/(1 + \varepsilon t), \quad t \geq 0, \quad F_\varepsilon := f_\varepsilon^\kappa(A),$$

for all $\varepsilon > 0$, and assume that H and F_ε , $\varepsilon > 0$, fulfill the hypotheses of Theorem 2.1, for some $m \in \mathbb{N} \cup \{\infty\}$. Then $\text{Ran}(H^{-n/2}) \subset \mathcal{D}(A^{\kappa n})$, for every $n \in \mathbb{N}$, $n < m + 1$, and

$$\|A^{\kappa n} H^{-n/2}\| \leq 4^{n-1} c^n \prod_{\ell=1}^{n-1} c_\ell.$$

If H and F_ε , $\varepsilon > 0$, fulfill the hypotheses of Corollary 2.2, then, for every $n \in \mathbb{N}$, $n < m$, it additionally follows that $A^{\kappa n} H^{-n/2}$ maps $\mathcal{D}(H)$ into itself so that $[A^{\kappa n}, H] H^{-n/2}$ is well-defined on $\mathcal{D}(H)$, and

$$\|[A^{\kappa n}, H] H^{-n/2}\| \leq 4^n c^{n-1} \prod_{\ell=1}^n c_\ell.$$

Proof. Let $U : \mathcal{H} \rightarrow L^2(\Omega, \mu)$ be a unitary transformation such that $a = U A U^*$ is a maximal operator of multiplication with some non-negative measurable function – again called a – on some measure space $(\Omega, \mathfrak{A}, \mu)$. We pick some $\psi \in \mathcal{H}$, set $\phi_n := U H^{-n/2} \psi$, and apply the monotone convergence

theorem to conclude that

$$\begin{aligned} \int_{\Omega} a(\omega)^{2\kappa n} |\phi_n(\omega)|^2 d\mu(\omega) &= \lim_{\varepsilon \searrow 0} \int_{\Omega} f_{\varepsilon}^{\kappa} (a(\omega))^{2n} |\phi_n(\omega)|^2 d\mu(\omega) \\ &= \lim_{\varepsilon \searrow 0} \|F_{\varepsilon}^n H^{-n/2} \psi\|^2 \leq C_n \|\psi\|^2, \end{aligned}$$

for every $n \in \mathbb{N}$, $n < m + 1$, which implies the first assertion. Now, assume that H and F_{ε} , $\varepsilon > 0$, fulfill Condition (c') of Corollary 2.2. Applying the dominated convergence theorem in the spectral representation introduced above we see that $F_{\varepsilon}^n \psi \rightarrow A^{\kappa n} \psi$, for every $\psi \in \mathcal{D}(A^{\kappa n})$. Hence, (2.7) and $\text{Ran}(H^{-n/2}) \subset \mathcal{D}(A^{\kappa n})$ imply, for $n < m$ and $\phi, \psi \in \mathcal{D}(H)$,

$$\begin{aligned} &|\langle \phi | A^{\kappa n} H^{-n/2} H \psi \rangle - \langle H \phi | A^{\kappa n} H^{-n/2} \psi \rangle| \\ &= \lim_{\varepsilon \searrow 0} |\langle F_{\varepsilon}^n \phi | H H^{-n/2} \psi \rangle - \langle H \phi | F_{\varepsilon}^n H^{-n/2} \psi \rangle| \\ &\leq \limsup_{\varepsilon \searrow 0} \|[F_{\varepsilon}^n, H] H^{-n/2}\| \|\phi\| \|\psi\| \leq C'_n \|\phi\| \|\psi\|. \end{aligned}$$

Thus, $|\langle H \phi | A^{\kappa n} H^{-n/2} \psi \rangle| \leq \|\phi\| \|A^{\kappa n} H^{-n/2}\| \|H \psi\| + C'_n \|\phi\| \|\psi\|$, for all $\phi, \psi \in \mathcal{D}(H)$. In particular, $A^{\kappa n} H^{-n/2} \psi \in \mathcal{D}(H^*) = \mathcal{D}(H)$, for all $\psi \in \mathcal{D}(H)$, and the second asserted bound holds true. \square

3. COMMUTATOR ESTIMATES

In this section we derive operator norm bounds on commutators involving the quantized vector potential, \mathbf{A} , the radiation field energy, H_f , and the Dirac operator, $D_{\mathbf{A}}$. The underlying Hilbert space is

$$\mathcal{H} := L^2(\mathbb{R}^3_{\mathbf{x}} \times \mathbb{Z}_4) \otimes \mathcal{F}_b = \int_{\mathbb{R}^3}^{\oplus} \mathbb{C}^4 \otimes \mathcal{F}_b d^3 \mathbf{x},$$

where the bosonic Fock space, \mathcal{F}_b , is modeled over the one-photon Hilbert space

$$\mathcal{F}_b^{(1)} := L^2(\mathcal{A} \times \mathbb{Z}_2, dk), \quad \int dk := \sum_{\lambda \in \mathbb{Z}_2} \int_{\mathcal{A}} d^3 \mathbf{k}.$$

With regards to the applications in [8] we define $\mathcal{A} := \{\mathbf{k} \in \mathbb{R}^3 : |\mathbf{k}| \geq m\}$, for some $m \geq 0$. We thus have

$$\mathcal{F}_b = \bigoplus_{n=0}^{\infty} \mathcal{F}_b^{(n)}, \quad \mathcal{F}_b^{(0)} := \mathbb{C}, \quad \mathcal{F}_b^{(n)} := \mathcal{S}_n L^2((\mathcal{A} \times \mathbb{Z}_2)^n), \quad n \in \mathbb{N},$$

where $\mathcal{S}_n = \mathcal{S}_n^2 = \mathcal{S}_n^*$ is given by

$$(\mathcal{S}_n \psi^{(n)})(k_1, \dots, k_n) := \frac{1}{n!} \sum_{\pi \in \mathfrak{S}_n} \psi^{(n)}(k_{\pi(1)}, \dots, k_{\pi(n)}),$$

for every $\psi^{(n)} \in L^2((\mathcal{A} \times \mathbb{Z}_2)^n)$, \mathfrak{S}_n denoting the group of permutations of $\{1, \dots, n\}$. The vector potential is determined by a certain vector-valued function, \mathbf{G} , called the form factor.

HYPOTHESIS 3.1. *The dispersion relation, $\omega : \mathcal{A} \rightarrow [0, \infty)$, is a measurable function such that $0 < \omega(k) := \omega(\mathbf{k}) \leq |\mathbf{k}|$, for $k = (\mathbf{k}, \lambda) \in \mathcal{A} \times \mathbb{Z}_2$ with $\mathbf{k} \neq 0$. For every $k \in (\mathcal{A} \setminus \{0\}) \times \mathbb{Z}_2$ and $j \in \{1, 2, 3\}$, $G^{(j)}(k)$ is a bounded continuously differentiable function, $\mathbb{R}_x^3 \ni \mathbf{x} \mapsto G_x^{(j)}(k)$, such that the map $(\mathbf{x}, k) \mapsto G_x^{(j)}(k)$ is measurable and $G_x^{(j)}(-\mathbf{k}, \lambda) = G_x^{(j)}(\mathbf{k}, \lambda)$, for almost every \mathbf{k} and all $\mathbf{x} \in \mathbb{R}^3$ and $\lambda \in \mathbb{Z}_2$. Finally, there exist $d_{-1}, d_0, d_1, \dots \in (0, \infty)$ such that*

$$(3.1) \quad 2 \int \omega(k)^\ell \|\mathbf{G}(k)\|_\infty^2 dk \leq d_\ell^2, \quad \ell \in \{-1, 0, 1, 2, \dots\},$$

$$(3.2) \quad 2 \int \omega(k)^{-1} \|\nabla_x \wedge \mathbf{G}(k)\|_\infty^2 dk \leq d_1^2,$$

where $\mathbf{G} = (G^{(1)}, G^{(2)}, G^{(3)})$ and $\|\mathbf{G}(k)\|_\infty := \sup_x |\mathbf{G}_x(k)|$, etc.

Example. In the physical applications the form factor is often given as

$$(3.3) \quad \mathbf{G}_x^{e,\Lambda}(k) := -e \frac{\mathbb{1}_{\{|\mathbf{k}| \leq \Lambda\}}}{2\pi\sqrt{|\mathbf{k}|}} e^{-i\mathbf{k} \cdot \mathbf{x}} \varepsilon(k),$$

for $(\mathbf{x}, k) \in \mathbb{R}^3 \times (\mathbb{R}^3 \times \mathbb{Z}_2)$ with $\mathbf{k} \neq 0$. Here the physical units are chosen such that energies are measured in units of the rest energy of the electron. Length are measured in units of one Compton wave length divided by 2π . The parameter $\Lambda > 0$ is an ultraviolet cut-off and the square of the elementary charge, $e > 0$, equals Sommerfeld's fine-structure constant in these units; we have $e^2 \approx 1/137$ in nature. The polarization vectors, $\varepsilon(\mathbf{k}, \lambda)$, $\lambda \in \mathbb{Z}_2$, are homogeneous of degree zero in \mathbf{k} such that $\{\mathring{\mathbf{k}}, \varepsilon(\mathring{\mathbf{k}}, 0), \varepsilon(\mathring{\mathbf{k}}, 1)\}$ is an orthonormal basis of \mathbb{R}^3 , for every $\mathring{\mathbf{k}} \in S^2$. This corresponds to the Coulomb gauge for $\nabla_x \cdot \mathbf{G}^{e,\Lambda} = 0$. We remark that the vector fields $S^2 \ni \mathring{\mathbf{k}} \mapsto \varepsilon(\mathring{\mathbf{k}}, \lambda)$ are necessarily discontinuous. \diamond

It is useful to work with more general form factors fulfilling Hypothesis 3.1 since in the study of the existence of ground states in QED one usually encounters truncated and discretized versions of the physical choice $\mathbf{G}^{e,\Lambda}$. For the applications in [8] it is necessary to know that the higher order estimates established here hold true uniformly in the involved parameters and Hypothesis 3.1 is convenient way to handle this.

We recall the definition of the creation and the annihilation operators of a photon state $f \in \mathcal{F}_b^{(1)}$,

$$(a^\dagger(f) \psi)^{(n)}(k_1, \dots, k_n) = n^{-1/2} \sum_{j=1}^n f(k_j) \psi^{(n-1)}(\dots, k_{j-1}, k_{j+1}, \dots), \quad n \in \mathbb{N},$$

$$(a(f) \psi)^{(n)}(k_1, \dots, k_n) = (n+1)^{1/2} \int \bar{f}(k) \psi^{(n+1)}(k, k_1, \dots, k_n) dk, \quad n \in \mathbb{N}_0,$$

and $(a^\dagger(f) \psi)^{(0)} = 0$, $a(f) (\psi^{(0)}, 0, 0, \dots) = 0$, for all $\psi = (\psi^{(n)})_{n=0}^\infty \in \mathcal{F}_b$ such that the right hand sides again define elements of \mathcal{F}_b . $a^\dagger(f)$ and $a(f)$ are

formal adjoints of each other on the dense domain

$$\mathcal{C}_0 := \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \mathcal{S}_n L_{\text{comp}}^{\infty}((\mathcal{A} \times \mathbb{Z}_2)^n). \quad (\text{Algebraic direct sum.})$$

For a three-vector of functions $\mathbf{f} = (f^{(1)}, f^{(2)}, f^{(3)}) \in (\mathcal{F}_b^{(1)})^3$, we write $a^{\sharp}(\mathbf{f}) := (a^{\sharp}(f^{(1)}), a^{\sharp}(f^{(2)}), a^{\sharp}(f^{(3)}))$, where a^{\sharp} is a^{\dagger} or a . Then the quantized vector potential is the triplet of operators given by

$$\mathbf{A} \equiv \mathbf{A}(\mathbf{G}) := a^{\dagger}(\mathbf{G}) + a(\mathbf{G}), \quad a^{\sharp}(\mathbf{G}) := \int_{\mathbb{R}^3}^{\oplus} \mathbb{1}_{\mathbb{C}^4} \otimes a^{\sharp}(\mathbf{G}_{\mathbf{x}}) d^3 \mathbf{x}.$$

The radiation field energy is the direct sum $H_f = \bigoplus_{n=0}^{\infty} d\Gamma^{(n)}(\omega) : \mathcal{D}(H_f) \subset \mathcal{F}_b \rightarrow \mathcal{F}_b$, where $d\Gamma^{(0)}(\omega) := 0$, and $d\Gamma^{(n)}(\omega)$ denotes the maximal multiplication operator in $\mathcal{F}_b^{(n)}$ associated with the symmetric function $(k_1, \dots, k_n) \mapsto \omega(k_1) + \dots + \omega(k_n)$. By the permutation symmetry and Fubini's theorem we thus have

$$(3.4) \quad \langle H_f^{1/2} \phi \mid H_f^{1/2} \psi \rangle = \int \omega(k) \langle a(k) \phi \mid a(k) \psi \rangle dk, \quad \phi, \psi \in \mathcal{D}(H_f^{1/2}),$$

where we use the notation

$$(a(k) \psi)^{(n)}(k_1, \dots, k_n) = (n + 1)^{1/2} \psi^{(n+1)}(k, k_1, \dots, k_n), \quad n \in \mathbb{N}_0,$$

almost everywhere, and $a(k) (\psi^{(0)}, 0, 0, \dots) = 0$. For a measurable function $f : \mathbb{R} \rightarrow \mathbb{R}$ and $\psi \in \mathcal{D}(f(H_f))$, the following identity in $\mathcal{F}_b^{(n)}$,

$$(a(k) f(H_f) \psi)^{(n)} = f(\omega(k) + d\Gamma^{(n)}(\omega)) (a(k) \psi)^{(n)}, \quad n \in \mathbb{N}_0,$$

valid for almost every k , is called the pull-through formula. Finally, we let $\alpha_1, \alpha_2, \alpha_3$, and $\beta := \alpha_0$ denote hermitian four times four matrices that fulfill the Clifford algebra relations

$$(3.5) \quad \alpha_i \alpha_j + \alpha_j \alpha_i = 2 \delta_{ij} \mathbb{1}, \quad i, j \in \{0, 1, 2, 3\}.$$

They act on the second tensor factor in $L^2(\mathbb{R}_{\mathbf{x}}^3 \times \mathbb{Z}_4) = L^2(\mathbb{R}_{\mathbf{x}}^3) \otimes \mathbb{C}^4$. As a consequence of (3.5) and the C^* -equality we have

$$(3.6) \quad \|\alpha \cdot \mathbf{v}\|_{\mathcal{L}(\mathbb{C}^4)} = |\mathbf{v}|, \quad \mathbf{v} \in \mathbb{R}^3, \quad \|\alpha \cdot \mathbf{z}\|_{\mathcal{L}(\mathbb{C}^4)} \leq \sqrt{2} |\mathbf{z}|, \quad \mathbf{z} \in \mathbb{C}^3,$$

where $\alpha \cdot \mathbf{z} := \alpha_1 z^{(1)} + \alpha_2 z^{(2)} + \alpha_3 z^{(3)}$, for $\mathbf{z} = (z^{(1)}, z^{(2)}, z^{(3)}) \in \mathbb{C}^3$. A standard exercise using the inequality in (3.6), the Cauchy-Schwarz inequality, and the canonical commutation relations,

$$[a^{\sharp}(f), a^{\sharp}(g)] = 0, \quad [a(f), a^{\dagger}(g)] = \langle f \mid g \rangle \mathbb{1}, \quad f, g \in \mathcal{F}_b^{(1)},$$

reveals that every $\psi \in \mathcal{D}(H_f^{1/2})$ belongs to the domain of $\alpha \cdot a^{\sharp}(\mathbf{G})$ and

$$(3.7) \quad \|\alpha \cdot a(\mathbf{G}) \psi\| \leq d_{-1} \|H_f^{1/2} \psi\|, \quad \|\alpha \cdot a^{\dagger}(\mathbf{G}) \psi\|^2 \leq d_{-1}^2 \|H_f^{1/2} \psi\|^2 + d_0^2 \|\psi\|^2.$$

(Here and in the following we identify $H_f \equiv \mathbb{1} \otimes H_f$, etc.) These relative bounds imply that $\alpha \cdot \mathbf{A}$ is symmetric on the domain $\mathcal{D}(H_f^{1/2})$.

The operators whose norms are estimated in (3.9) and the following lemmata are always well-defined a priori on the following dense subspace of \mathcal{H} ,

$$\mathcal{D} := C_0^\infty(\mathbb{R}^3 \times \mathbb{Z}_4) \otimes \mathcal{C}_0. \quad (\text{Algebraic tensor product.})$$

Given some $E \geq 1$ we set

$$(3.8) \quad \check{H}_f := H_f + E$$

in the sequel. We already know from [10] that, for every $\nu \geq 0$, there is some constant, $C_\nu \in (0, \infty)$, such that

$$(3.9) \quad \| [\boldsymbol{\alpha} \cdot \mathbf{A}, \check{H}_f^{-\nu}] \check{H}_f^\nu \| \leq C_\nu / E^{1/2}, \quad E \geq 1.$$

In our first lemma we derive a generalization of (3.9). Its proof resembles the one of (3.9) given in [10]. Since we shall encounter many similar but slightly different commutators in the applications it makes sense to introduce the numerous parameters that obscure its statement (but simplify its proof).

LEMMA 3.2. *Assume that ω and \mathbf{G} fulfill Hypothesis 3.1. Let $\varepsilon \geq 0$, $E \geq 1$, $\kappa, \nu \in \mathbb{R}$, $\gamma, \delta, \sigma, \tau \geq 0$, such that $\gamma + \delta + \sigma + \tau \leq 1/2$, and define*

$$(3.10) \quad f_\varepsilon(t) := \frac{t + E}{1 + \varepsilon t + \varepsilon E}, \quad t \in [0, \infty).$$

Then the operator $\check{H}_f^{\nu+\gamma} f_\varepsilon^\sigma(H_f) [\boldsymbol{\alpha} \cdot \mathbf{A}, f_\varepsilon^\kappa(H_f)] \check{H}_f^{-\nu+\delta} f_\varepsilon^{-\kappa+\tau}(H_f)$, defined a priori on \mathcal{D} , extends to a bounded operator on \mathcal{H} and

$$(3.11) \quad \begin{aligned} & \| \check{H}_f^{\nu+\gamma} f_\varepsilon^\sigma(H_f) [\boldsymbol{\alpha} \cdot \mathbf{A}, f_\varepsilon^\kappa(H_f)] \check{H}_f^{-\nu+\delta} f_\varepsilon^{-\kappa+\tau}(H_f) \| \\ & \leq |\kappa| 2^{(\rho+1)/2} (d_1 + d_\rho) E^{\gamma+\delta+\sigma+\tau-1/2}, \end{aligned}$$

where ρ is the smallest integer greater or equal to $3 + 2|\kappa| + 2|\nu|$.

Proof. We notice that all operators \check{H}_f^s and $f_\varepsilon^s(H_f)$ leave the dense subspace \mathcal{D} invariant and that $\boldsymbol{\alpha} \cdot a^\sharp(\mathbf{G})$ maps \mathcal{D} into $\mathcal{D}(\check{H}_f^s)$, for every $s \in \mathbb{R}$. Now, let $\varphi, \psi \in \mathcal{D}$. Then

$$(3.12) \quad \begin{aligned} & \langle \varphi | \check{H}_f^{\nu+\gamma} f_\varepsilon^\sigma(H_f) [\boldsymbol{\alpha} \cdot \mathbf{A}, f_\varepsilon^\kappa(H_f)] \check{H}_f^{-\nu+\delta} f_\varepsilon^{-\kappa+\tau}(H_f) \psi \rangle \\ & = \langle \varphi | \check{H}_f^{\nu+\gamma} f_\varepsilon^\sigma(H_f) [\boldsymbol{\alpha} \cdot a(\mathbf{G}), f_\varepsilon^\kappa(H_f)] \check{H}_f^{-\nu+\delta} f_\varepsilon^{-\kappa+\tau}(H_f) \psi \rangle \\ (3.13) \quad & - \langle f_\varepsilon^{-\kappa+\tau}(H_f) \check{H}_f^{-\nu+\delta} [\boldsymbol{\alpha} \cdot a(\mathbf{G}), f_\varepsilon^\kappa(H_f)] f_\varepsilon^\sigma(H_f) \check{H}_f^{\nu+\gamma} \varphi | \psi \rangle. \end{aligned}$$

For almost every k , the pull-through formula yields the following representation,

$$\check{H}_f^{\nu+\gamma} f_\varepsilon^\sigma(H_f) [a(k), f_\varepsilon^\kappa(H_f)] \check{H}_f^{-\nu+\delta} f_\varepsilon^{-\kappa+\tau}(H_f) \psi = F(k; H_f) a(k) \check{H}_f^{-1/2} \psi,$$

where

$$\begin{aligned} F(k; t) &:= (t + E)^{\nu+\gamma} f_\varepsilon^\sigma(t) (f_\varepsilon^\kappa(t + \omega(k)) - f_\varepsilon^\kappa(t)) \\ &\quad \cdot (t + E + \omega(k))^{-\nu+\delta+1/2} f_\varepsilon^{-\kappa+\tau}(t + \omega(k)) \\ &= \left(\frac{t + E}{t + E + \omega(k)} \right)^\nu (t + E)^\gamma (t + E + \omega(k))^{\delta+1/2} \\ &\quad \cdot \int_0^1 \frac{d}{ds} f_\varepsilon^\kappa(t + s\omega(k)) ds \frac{f_\varepsilon^\sigma(t) f_\varepsilon^\tau(t + \omega(k))}{f_\varepsilon^\kappa(t + \omega(k))}, \end{aligned}$$

for $t \geq 0$. We compute

$$(3.14) \quad \frac{d}{ds} f_\varepsilon^\kappa(t + s\omega(k)) = \frac{\kappa \omega(k) f_\varepsilon^\kappa(t + s\omega(k))}{(t + s\omega(k) + E)(1 + \varepsilon t + \varepsilon s\omega(k) + \varepsilon E)}.$$

Using that f_ε is increasing in $t \geq 0$ and that

$$(t + \omega(k) + E)/(t + s\omega(k) + E) \leq 1 + \omega(k), \quad s \in [0, 1],$$

thus

$$f_\varepsilon^\kappa(t + s\omega(k))/f_\varepsilon^\kappa(t + \omega(k)) \leq (1 + \omega(k))^{-(0 \wedge \kappa)}, \quad s \in [0, 1],$$

it is elementary to verify that

$$|F_\varepsilon(k; t)| \leq |\kappa| \omega(k) (1 + \omega(k))^{\delta+\tau-(0 \wedge \kappa)-(0 \wedge \nu)+1/2} E^{\gamma+\delta+\sigma+\tau-1/2},$$

for all $t \geq 0$ and k . We deduce that the term in (3.12) can be estimated as

$$\begin{aligned} &|\langle \varphi | \check{H}_f^{\nu+\gamma} f_\varepsilon^\sigma(H_f) [\boldsymbol{\alpha} \cdot a(\mathbf{G}), f_\varepsilon^\kappa(H_f)] \check{H}_f^{-\nu+\delta} f_\varepsilon^{-\kappa+\tau}(H_f) \psi \rangle| \\ &\leq \int \|\varphi\| \|\boldsymbol{\alpha} \cdot \mathbf{G}(k) \check{H}_f^{\nu+\gamma} f_\varepsilon^\sigma(H_f) [a(k), f_\varepsilon^\kappa(H_f)] \check{H}_f^{-\nu+\delta} f_\varepsilon^{-\kappa+\tau}(H_f) \psi\| dk \\ &\leq \sqrt{2} \int \|\varphi\| \|\mathbf{G}(k)\|_\infty \|F_\varepsilon(k; H_f)\| \|a(k) \check{H}_f^{-1/2} \psi\| dk \\ &\leq |\kappa| \sqrt{2} \left(\int \omega(k) (1 + \omega(k))^{2(\delta+\tau)-(0 \wedge 2\kappa)-(0 \wedge 2\nu)+1} \|\mathbf{G}(k)\|_\infty^2 dk \right)^{1/2} \\ &\quad \cdot \left(\int \omega(k) \|a(k) \check{H}_f^{-1/2} \psi\|^2 dk \right)^{1/2} \|\varphi\| E^{\gamma+\delta+\sigma+\tau-1/2} \\ (3.15) \quad &\leq |\kappa| 2^{(\rho-1)/2} (d_1 + d_\rho) \|\varphi\| \|H_f^{1/2} \check{H}_f^{-1/2} \psi\| E^{\gamma+\delta+\sigma+\tau-1/2}. \end{aligned}$$

In the last step we used $\delta + \tau \leq 1/2$ and applied (3.4). (3.15) immediately gives a bound on the term in (3.13), too. For we have

$$\begin{aligned} &f_\varepsilon^{-\kappa+\tau}(H_f) \check{H}_f^{-\nu+\delta} [\boldsymbol{\alpha} \cdot a(\mathbf{G}), f_\varepsilon^\kappa(H_f)] f_\varepsilon^\sigma(H_f) \check{H}_f^{\nu+\gamma} \varphi \\ &= \check{H}_f^{-\nu+\delta} f_\varepsilon^\tau(H_f) [f_\varepsilon^{-\kappa}(H_f), \boldsymbol{\alpha} \cdot a(\mathbf{G})] \check{H}_f^{\nu+\gamma} f_\varepsilon^{\kappa+\sigma}(H_f) \varphi, \end{aligned}$$

which after the replacements $(\nu, \kappa, \gamma, \delta, \sigma, \tau) \mapsto (-\nu, -\kappa, \delta, \gamma, \tau, \sigma)$ and $\varphi \mapsto -\psi$ is precisely the term we just have treated. \square

Lemma 3.2 provides all the information needed to apply Corollary 2.3 to non-relativistic QED. For the application of Corollary 2.3 to the non-local semi-relativistic models of QED it is necessary to study commutators that involve resolvents and sign functions of the Dirac operator,

$$D_{\mathbf{A}} := \boldsymbol{\alpha} \cdot (-i\nabla_{\mathbf{x}} + \mathbf{A}) + \beta.$$

An application of Nelson’s commutator theorem with test operator $-\Delta + H_f + 1$ shows that $D_{\mathbf{A}}$ is essentially self-adjoint on \mathcal{D} . The spectrum of its unique closed extension, again denoted by the same symbol, is contained in the union of two half-lines, $\sigma[D_{\mathbf{A}}] \subset (-\infty, -1] \cup [1, \infty)$. In particular, it makes sense to define

$$R_{\mathbf{A}}(iy) := (D_{\mathbf{A}} - iy)^{-1}, \quad y \in \mathbb{R},$$

and the spectral calculus yields

$$\|R_{\mathbf{A}}(iy)\| \leq (1 + y^2)^{-1/2}, \quad \int_{\mathbb{R}} \| |D_{\mathbf{A}}|^{1/2} R_{\mathbf{A}}(iy) \psi \|^2 \frac{dy}{\pi} = \|\psi\|^2, \quad \psi \in \mathcal{H}.$$

The next lemma is a straightforward extension of [10, Corollary 3.1] where it is also shown that $R_{\mathbf{A}}(iy)$ maps $\mathcal{D}(H_f^\nu)$ into itself, for every $\nu > 0$.

LEMMA 3.3. *Assume that ω and \mathbf{G} fulfill Hypothesis 3.1. Then, for all $\kappa, \nu \in \mathbb{R}$, we find $k_i \equiv k_i(\kappa, \nu, d_1, d_\rho) \in [1, \infty)$, $i = 1, 2$, such that, for all $y \in \mathbb{R}$, $\varepsilon \geq 0$, and $E \geq k_1$, there exist $\Upsilon_{\kappa, \nu}(iy), \tilde{\Upsilon}_{\kappa, \nu}(iy) \in \mathcal{L}(\mathcal{H})$ satisfying*

$$(3.16) \quad R_{\mathbf{A}}(iy) \check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f) = \check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f) R_{\mathbf{A}}(iy) \Upsilon_{\kappa, \nu}(iy)$$

$$(3.17) \quad = \check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f) \tilde{\Upsilon}_{\kappa, \nu}(iy) R_{\mathbf{A}}(iy),$$

on $\mathcal{D}(\check{H}_f^{-\nu})$, and $\|\Upsilon_{\kappa, \nu}(iy)\|, \|\tilde{\Upsilon}_{\kappa, \nu}(iy)\| \leq k_2$, where ρ is defined in Lemma 3.2.

Proof. Without loss of generality we may assume that $\varepsilon > 0$ for otherwise we could simply replace ν by $\nu + \kappa$ and f_0^κ by $f_0^0 = 1$. First, we assume in addition that $\nu \geq 0$. We observe that

$$T_0 := [\check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f), \boldsymbol{\alpha} \cdot \mathbf{A}] \check{H}_f^\nu f_\varepsilon^\kappa(H_f) = T_1 + T_2$$

on \mathcal{D} , where

$$T_1 := [\check{H}_f^{-\nu}, \boldsymbol{\alpha} \cdot \mathbf{A}] \check{H}_f^\nu, \quad T_2 := \check{H}_f^{-\nu} [f_\varepsilon^{-\kappa}(H_f), \boldsymbol{\alpha} \cdot \mathbf{A}] f_\varepsilon^\kappa(H_f) \check{H}_f^\nu.$$

Due to (3.9) (or (3.11) with $\varepsilon = 0$) the operator T_1 extends to a bounded operator on \mathcal{H} and $\|T_1\| \leq C_\nu/E^{1/2}$. According to (3.11) we further have $\|T_2\| \leq C_{\kappa, \nu}(d_1 + d_\rho)/E^{1/2}$. We pick some $\phi \in \mathcal{D}$ and compute

$$(3.18) \quad \begin{aligned} [R_{\mathbf{A}}(iy), \check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f)] (D_{\mathbf{A}} - iy) \phi &= R_{\mathbf{A}}(iy) [\check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f), D_{\mathbf{A}}] \phi \\ &= R_{\mathbf{A}}(iy) T_0 \check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f) \phi \\ &= R_{\mathbf{A}}(iy) \bar{T}_0 \check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f) R_{\mathbf{A}}(iy) (D_{\mathbf{A}} - iy) \phi. \end{aligned}$$

Since $(D_{\mathbf{A}} - iy) \mathcal{D}$ is dense in \mathcal{H} and since $\check{H}_f^{-\nu}$ and $f_\varepsilon^\kappa(H_f)$ are bounded (here we use that $\nu \geq 0$ and $\varepsilon > 0$), this identity implies

$$R_{\mathbf{A}}(iy) \check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f) = (\mathbb{1} + R_{\mathbf{A}}(iy) \bar{T}_0) \check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f) R_{\mathbf{A}}(iy).$$

Taking the adjoint of the previous identity and replacing y by $-y$ we obtain

$$\check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f) R_{\mathbf{A}}(iy) = R_{\mathbf{A}}(iy) \check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f) (\mathbb{1} + T_0^* R_{\mathbf{A}}(iy)).$$

In view of the norm bounds on T_1 and T_2 we see that (3.16) and (3.17) are valid with $\Upsilon_{\kappa,\nu}(iy) := \sum_{\ell=0}^\infty \{-T_0^* R_{\mathbf{A}}(iy)\}^\ell$ and $\tilde{\Upsilon}_{\kappa,\nu}(iy) := \sum_{\ell=0}^\infty \{-R_{\mathbf{A}}(iy) T_0^*\}^\ell$, provided that E is sufficiently large, depending only on κ, ν, d_1 , and d_ρ , such that the Neumann series converge.

Now, let $\nu < 0$. Then we write T_0 on the domain \mathcal{D} as

$$T_0 = \check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f) [\boldsymbol{\alpha} \cdot \mathbf{A}, \check{H}_f^\nu f_\varepsilon^\kappa(H_f)],$$

and deduce that

$$R_{\mathbf{A}}(iy) \check{H}_f^\nu f_\varepsilon^\kappa(H_f) (\mathbb{1} + \bar{T}_0 R_{\mathbf{A}}(iy)) = \check{H}_f^\nu f_\varepsilon^\kappa(H_f) R_{\mathbf{A}}(iy)$$

by a computation analogous to (3.18). Taking the adjoint of this identity with y replaced by $-y$ we get

$$(\mathbb{1} + R_{\mathbf{A}}(iy) T_0^*) \check{H}_f^\nu f_\varepsilon^\kappa R_{\mathbf{A}}(iy) = R_{\mathbf{A}}(iy) \check{H}_f^\nu f_\varepsilon^\kappa(H_f).$$

Next, we invert $\mathbb{1} + R_{\mathbf{A}}(iy) T_0^*$ by means of the same Neumann series as above. As a result we obtain

$$\check{H}_f^\nu f_\varepsilon^\kappa(H_f) R_{\mathbf{A}}(iy) = R_{\mathbf{A}}(iy) \Upsilon_{\kappa,\nu}(iy) \check{H}_f^\nu f_\varepsilon^\kappa(H_f) = \tilde{\Upsilon}_{\kappa,\nu}(iy) R_{\mathbf{A}}(iy) \check{H}_f^\nu f_\varepsilon^\kappa(H_f),$$

where the definition of $\Upsilon_{\kappa,\nu}$ and $\tilde{\Upsilon}_{\kappa,\nu}$ has been extended to negative ν . It follows that $R_{\mathbf{A}}(iy) \Upsilon_{\kappa,\nu}(iy) = \tilde{\Upsilon}_{\kappa,\nu}(iy) R_{\mathbf{A}}(iy)$ maps $\mathcal{D}(\check{H}_f^{-\nu}) = \mathcal{D}(\check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f)) = \text{Ran}(\check{H}_f^\nu f_\varepsilon^\kappa(H_f))$ into itself and that (3.16) and (3.17) still hold true when ν is negative. \square

In order to control the Coulomb singularity $1/|\mathbf{x}|$ in terms of $|D_{\mathbf{A}}|$ and H_f in the proof of the following corollary, we shall employ the bound [10, Theorem 2.3]

$$(3.19) \quad \frac{2}{\pi} \frac{1}{|\mathbf{x}|} \leq |D_{\mathbf{A}}| + H_f + k d_1^2,$$

which holds true in sense of quadratic forms on $\mathcal{Q}(|D_{\mathbf{A}}|) \cap \mathcal{Q}(H_f)$. Here $k \in (0, \infty)$ is some universal constant. We abbreviate the sign function of the Dirac operator, which can be represented as a strongly convergent principal value [6, Lemma VI.5.6], by

$$(3.20) \quad S_{\mathbf{A}} \psi := D_{\mathbf{A}} |D_{\mathbf{A}}|^{-1} \psi = \lim_{\tau \rightarrow \infty} \int_{-\tau}^{\tau} R_{\mathbf{A}}(iy) \psi \frac{dy}{\pi}.$$

We recall from [10, Lemma 3.3] that $S_{\mathbf{A}}$ maps $\mathcal{D}(H_f^\nu)$ into itself, for every $\nu > 0$. This can also be read off from the proof of the next corollary.

COROLLARY 3.4. *Assume that ω and \mathbf{G} fulfill Hypothesis 3.1. Let $\kappa, \nu \in \mathbb{R}$. Then we find some $C \equiv C(\kappa, \nu, d_1, d_\rho) \in (0, \infty)$ such that, for all $\gamma, \delta, \sigma, \tau \geq 0$*

with $\gamma + \delta + \sigma + \tau \leq 1/2$ and all $\varepsilon \geq 0$, $E \geq k_1$,

$$(3.21) \quad \left\| \check{H}_f^\nu f_\varepsilon^\kappa(H_f) S_{\mathbf{A}} \check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f) \right\| \leq C,$$

$$(3.22) \quad \left\| |D_{\mathbf{A}}|^{1/2} \check{H}_f^{\nu+\gamma} f_\varepsilon^\sigma(H_f) [S_{\mathbf{A}}, f_\varepsilon^\kappa(H_f)] \check{H}_f^{-\nu+\delta} f_\varepsilon^{-\kappa+\tau}(H_f) \right\| \leq C,$$

$$(3.23) \quad \left\| |\mathbf{x}|^{-1/2} \check{H}_f^\nu f_\varepsilon^\sigma(H_f) [S_{\mathbf{A}}, f_\varepsilon^\kappa(H_f)] \check{H}_f^{-\nu-\sigma-\tau} f_\varepsilon^{-\kappa+\tau}(H_f) \right\| \leq C.$$

(k_1 is the constant appearing in Lemma 3.3, \check{H}_f is given by (3.8), f_ε by (3.10).)

Proof. First, we prove (3.22). Using (3.20), writing

$$[R_{\mathbf{A}}(iy), f_\varepsilon^\kappa(H_f)] = R_{\mathbf{A}}(iy) [f_\varepsilon^\kappa(H_f), \boldsymbol{\alpha} \cdot \mathbf{A}] R_{\mathbf{A}}(iy)$$

on \mathcal{D} and employing (3.16), (3.17), and (3.11) we obtain the following estimate, for all $\varphi, \psi \in \mathcal{D}$, and $E \geq k_1$,

$$\begin{aligned} & \left| \left\langle |D_{\mathbf{A}}|^{1/2} \varphi \left| \check{H}_f^{\nu+\gamma} f_\varepsilon^\sigma(H_f) [S_{\mathbf{A}}, f_\varepsilon^\kappa(H_f)] \check{H}_f^{-\nu+\delta} f_\varepsilon^{-\kappa+\tau} \psi \right. \right\rangle \right| \\ & \leq \int_{\mathbb{R}} \left| \left\langle \check{H}_f^{\nu+\gamma} |D_{\mathbf{A}}|^{1/2} \varphi \left| f_\varepsilon^\sigma(H_f) [f_\varepsilon^\kappa(H_f), R_{\mathbf{A}}(iy)] \times \right. \right. \right. \\ & \quad \left. \left. \left. \times \check{H}_f^{-\nu+\delta} f_\varepsilon^{-\kappa+\tau}(H_f) \psi \right. \right\rangle \right| \frac{dy}{\pi} \\ & = \int_{\mathbb{R}} \left| \left\langle \varphi \left| |D_{\mathbf{A}}|^{1/2} R_{\mathbf{A}}(iy) \Upsilon_{\sigma, \nu+\gamma}(iy) \check{H}_f^{\nu+\gamma} f_\varepsilon^\sigma(H_f) [f_\varepsilon^\kappa(H_f), \boldsymbol{\alpha} \cdot \mathbf{A}] \times \right. \right. \right. \\ & \quad \left. \left. \left. \times \check{H}_f^{-\nu+\delta} f_\varepsilon^{-\kappa+\tau}(H_f) \tilde{\Upsilon}_{\kappa-\tau, \nu-\delta}(iy) R_{\mathbf{A}}(iy) \psi \right. \right\rangle \right| \frac{dy}{\pi} \\ & \leq C_{\kappa, \nu} (d_1 + d_\rho) E^{\gamma+\delta+\sigma+\tau-1/2} \sup_{y \in \mathbb{R}} \{ \|\Upsilon_{\sigma, \nu+\gamma}(iy)\| \|\tilde{\Upsilon}_{\kappa-\tau, \nu-\delta}(iy)\| \} \\ & \quad \cdot \left(\int_{\mathbb{R}} \| |D_{\mathbf{A}}|^{1/2} R_{\mathbf{A}}(iy) \varphi \|^2 \frac{dy}{\pi} \right)^{1/2} \left(\int_{\mathbb{R}} \| R_{\mathbf{A}}(iy) \psi \|^2 \frac{dy}{\pi} \right)^{1/2} \\ & \leq C_{\kappa, \nu, d_1, d_\rho} E^{\gamma+\delta+\sigma+\tau-1/2} \|\varphi\| \|\psi\|. \end{aligned}$$

This estimate shows that the vector in the right entry of the scalar product in the first line belongs to $\mathcal{D}((|D_{\mathbf{A}}|^{1/2})^*) = \mathcal{D}(|D_{\mathbf{A}}|^{1/2})$ and that (3.22) holds true. Next, we observe that (3.23) follows from (3.22) and (3.19). Finally, (3.21) follows from $\|X\| \leq \text{const}(\nu, \kappa, d_1, d_\rho)$, where $X := \check{H}_f^\nu f_\varepsilon^\kappa(H_f) [S_{\mathbf{A}}, \check{H}_f^{-\nu} f_\varepsilon^{-\kappa}(H_f)]$. Such a bound on $\|X\|$ is, however, an immediate consequence of (3.22) (where we can choose $\varepsilon = 0$) because

$$X = [\check{H}_f^\nu, S_{\mathbf{A}}] \check{H}_f^{-\nu} + \check{H}_f^\nu [f_\varepsilon^\kappa(H_f), S_{\mathbf{A}}] f_\varepsilon^{-\kappa}(H_f) \check{H}_f^{-\nu}$$

on the domain \mathcal{D} . □

4. NON-RELATIVISTIC QED

The Pauli-Fierz operator for a molecular system with static nuclei and $N \in \mathbb{N}$ electrons interacting with the quantized radiation field is acting in the Hilbert space

$$(4.1) \quad \mathcal{H}_N := \mathcal{A}_N L^2((\mathbb{R}^3 \times \mathbb{Z}_4)^N) \otimes \mathcal{F}_{\mathbf{b}},$$

where $\mathcal{A}_N = \mathcal{A}_N^2 = \mathcal{A}_N^*$ denotes anti-symmetrization,

$$(\mathcal{A}_N \Psi)(X) := \frac{1}{N!} \sum_{\pi \in \mathfrak{S}_N} (-1)^\pi \Psi(\mathbf{x}_{\pi(1)}, \varsigma_{\pi(1)}, \dots, \mathbf{x}_{\pi(N)}, \varsigma_{\pi(N)}),$$

for $\Psi \in L^2((\mathbb{R}^3 \times \mathbb{Z}_4)^N)$ and a.e. $X = (\mathbf{x}_i, \varsigma_i)_{i=1}^N \in (\mathbb{R}^3 \times \mathbb{Z}_4)^N$. a priori it is defined on the dense domain

$$\mathcal{D}_N := \mathcal{A}_N C_0^\infty((\mathbb{R}^3 \times \mathbb{Z}_4)^N) \otimes \mathcal{C}_0,$$

the tensor product understood in the algebraic sense, by

$$(4.2) \quad H_{\text{nr}}^V \equiv H_{\text{nr}}^V(\mathbf{G}) := \sum_{i=1}^N (D_{\mathbf{A}}^{(i)})^2 + V + H_f.$$

A superscript (i) indicates that the operator below is acting on the pair of variables $(\mathbf{x}_i, \varsigma_i)$. In fact, the operator defined in (4.2) is a two-fold copy of the usual Pauli-Fierz operator which acts on two-spinors and the energy has been shifted by N in (4.2). For (3.5) implies

$$(4.3) \quad D_{\mathbf{A}}^2 = \mathcal{T}_{\mathbf{A}} \oplus \mathcal{T}_{\mathbf{A}}, \quad \mathcal{T}_{\mathbf{A}} := (\boldsymbol{\sigma} \cdot (-i\nabla_{\mathbf{x}} + \mathbf{A}))^2 + 1.$$

Here $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is a vector containing the Pauli matrices (when $\alpha_j, j \in \{0, 1, 2, 3\}$, are given in Dirac's standard representation). We write H_{nr}^V in the form (4.2) to maintain a unified notation throughout this paper.

We shall only make use of the following properties of the potential V .

HYPOTHESIS 4.1. *V can be written as $V = V_+ - V_-$, where $V_{\pm} \geq 0$ is a symmetric operator acting in $\mathcal{A}_N L^2((\mathbb{R}^3 \times \mathbb{Z}_4)^4)$ such that $\mathcal{D}_N \subset \mathcal{D}(V_{\pm})$. There exist $a \in (0, 1)$ and $b \in (0, \infty)$ such that $V_- \leq a H_{\text{nr}}^0 + b$ in the sense of quadratic forms on \mathcal{D}_N .*

Example. The Coulomb potential generated by $K \in \mathbb{N}$ fixed nuclei located at the positions $\{\mathbf{R}_1, \dots, \mathbf{R}_K\} \subset \mathbb{R}^3$ is given as

$$(4.4) \quad V_C(X) := - \sum_{i=1}^N \sum_{k=1}^K \frac{e^2 Z_k}{|\mathbf{x}_i - \mathbf{R}_k|} + \sum_{\substack{i,j=1 \\ i < j}}^N \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|},$$

for some $e, Z_1, \dots, Z_K > 0$ and a.e. $X = (\mathbf{x}_i, \varsigma_i)_{i=1}^N \in (\mathbb{R}^3 \times \mathbb{Z}_4)^N$. It is well-known that V_C is infinitesimally H_{nr}^0 -bounded and that V_C fulfills Hypothesis 4.1. ◊

It follows immediately from Hypothesis 4.1 that H_{nr}^V has a self-adjoint Friedrichs extension – henceforth denoted by the same symbol H_{nr}^V – and that \mathcal{D}_N is a form core for H_{nr}^V . Moreover, we have

$$(4.5) \quad (D_{\mathbf{A}}^{(1)})^2, \dots, (D_{\mathbf{A}}^{(N)})^2, V_+, H_f \leq H_{\text{nr}}^{V_+} \leq (1 - a)^{-1} (H_{\text{nr}}^V + b)$$

on \mathcal{D}_N . In [4] it is shown that $\mathcal{D}((H_{\text{nr}}^V)^{n/2}) \subset \mathcal{D}(H_f^{n/2})$, for every $n \in \mathbb{N}$. We re-derive this result by means of Corollary 2.3 in the next theorem where

$$E_{\text{nr}} := \inf \sigma[H_{\text{nr}}^V], \quad H'_{\text{nr}} := H_{\text{nr}}^V - E_{\text{nr}} + 1.$$

THEOREM 4.2. Assume that ω and \mathbf{G} fulfill Hypothesis 3.1 and that V fulfills Hypothesis 4.1. Assume in addition that

$$(4.6) \quad 2 \int \omega(k)^\ell \|\nabla_{\mathbf{x}} \wedge \mathbf{G}(k)\|_\infty^2 dk \leq d_{\ell+2}^2,$$

$$(4.7) \quad \int \omega(k)^\ell \|\nabla_{\mathbf{x}} \cdot \mathbf{G}(k)\|_\infty^2 dk \leq d_{\ell+2}^2,$$

for all $\ell \in \{-1, 0, 1, 2, \dots\}$. Then, for every $n \in \mathbb{N}$, we have $\mathcal{D}((H_{\text{nr}}^V)^{n/2}) \subset \mathcal{D}(H_{\text{f}}^{n/2})$, $H_{\text{f}}^{n/2} (H_{\text{nr}}')^{-n/2}$ maps $\mathcal{D}(H_{\text{nr}}^V)$ into itself, and

$$\begin{aligned} \|H_{\text{f}}^{n/2} (H_{\text{nr}}')^{-n/2}\| &\leq C(N, n, a, b, d_{-1}, d_1, d_{5+n}) (|E_{\text{nr}}| + 1)^{(3n-2)/2}, \\ \|[H_{\text{f}}^{n/2}, H_{\text{nr}}^V] (H_{\text{nr}}')^{-n/2}\| &\leq C'(N, n, a, b, d_{-1}, d_1, d_{5+n}) (|E_{\text{nr}}| + 1)^{(3n-1)/2}. \end{aligned}$$

Proof. We pick the function f_ε defined in (3.10) with $E = 1$ and verify that the operators $F_\varepsilon^n := f_\varepsilon^{n/2}(H_{\text{f}})$, $\varepsilon > 0$, $n \in \mathbb{N}$, and H_{nr}' fulfill the conditions (a), (b), and (c') of Theorem 2.1 and Corollary 2.2 with $m = \infty$. Then the assertion follows from Corollary 2.3. We set $\check{H}_{\text{f}} := H_{\text{f}} + E$ in what follows. By means of (4.5) we find

$$(4.8) \quad \langle \Psi | F_\varepsilon^2 \Psi \rangle \leq \langle \Psi | \check{H}_{\text{f}} \Psi \rangle \leq \frac{E_{\text{nr}} + b + E}{1 - a} \langle \Psi | H_{\text{nr}}' \Psi \rangle,$$

for all $\Psi \in \mathcal{D}_N$, which is Condition (b). Next, we observe that F_ε maps \mathcal{D}_N into itself. Employing (4.5) once more and using $-V_- \leq 0$ and the fact that $V_+ \geq 0$ and F_ε act on different tensor factors we deduce that

$$(4.9) \quad \begin{aligned} \langle F_\varepsilon \Psi | (V + H_{\text{f}}) F_\varepsilon \Psi \rangle &\leq \|f_\varepsilon\|_\infty \langle \Psi | (V_+ + H_{\text{f}}) \Psi \rangle \\ &\leq \|f_\varepsilon\|_\infty \frac{E_{\text{nr}} + b + E}{1 - a} \langle \Psi | H_{\text{nr}}' \Psi \rangle, \end{aligned}$$

for every $\Psi \in \mathcal{D}_N$. Thanks to (3.11) with $\kappa = 1/2$, $\nu = \gamma = \delta = \sigma = \tau = 0$, and (4.5) we further find some $C \in (0, \infty)$ such that

$$(4.10) \quad \begin{aligned} \|D_{\mathbf{A}}^{(i)} F_\varepsilon \Psi\|^2 &\leq 2 \|f_\varepsilon\|_\infty \|D_{\mathbf{A}}^{(i)} \Psi\|^2 + 2 \|f_\varepsilon\|_\infty \|F_\varepsilon^{-1} [\boldsymbol{\alpha} \cdot \mathbf{A}, F_\varepsilon]\|^2 \|\Psi\|^2 \\ &\leq C \|f_\varepsilon\|_\infty \langle \Psi | H_{\text{nr}}' \Psi \rangle, \end{aligned}$$

for all $\Psi \in \mathcal{D}_N$. (4.9) and (4.10) together show that Condition (a) is fulfilled, too. Finally, we verify the bound in (c'). We use

$$[\boldsymbol{\alpha} \cdot (-i\nabla_{\mathbf{x}}), \boldsymbol{\alpha} \cdot \mathbf{A}] = \boldsymbol{\Sigma} \cdot \mathbf{B} - i(\nabla_{\mathbf{x}} \cdot \mathbf{A}),$$

where $\mathbf{B} := a^\dagger(\nabla_{\mathbf{x}} \wedge \mathbf{G}) + a(\nabla_{\mathbf{x}} \wedge \mathbf{G})$ is the magnetic field and the j -th entry of the formal vector $\boldsymbol{\Sigma}$ is $-i\epsilon_{jkl} \alpha_k \alpha_\ell$, $j, k, \ell \in \{1, 2, 3\}$, to write the square of the Dirac operator on the domain \mathcal{D} as

$$D_{\mathbf{A}}^2 = D_0^2 + \boldsymbol{\Sigma} \cdot \mathbf{B} - i(\nabla_{\mathbf{x}} \cdot \mathbf{A}) + (\boldsymbol{\alpha} \cdot \mathbf{A})^2 + 2\boldsymbol{\alpha} \cdot \mathbf{A} \boldsymbol{\alpha} \cdot (-i\nabla_{\mathbf{x}}).$$

This yields

$$[H'_{\text{nr}}, F_\varepsilon^n] = \sum_{i=1}^N [(D_{\mathbf{A}}^{(i)})^2, F_\varepsilon^n] = \sum_{i=1}^N \{ [\boldsymbol{\Sigma} \cdot \mathbf{B}^{(i)}, F_\varepsilon^n] - i [(\nabla_{\mathbf{x}} \cdot \mathbf{A}^{(i)}), F_\varepsilon^n] + \boldsymbol{\alpha} \cdot \mathbf{A}^{(i)} [\boldsymbol{\alpha} \cdot \mathbf{A}^{(i)}, F_\varepsilon^n] + [\boldsymbol{\alpha} \cdot \mathbf{A}^{(i)}, F_\varepsilon^n] (2D_{\mathbf{A}}^{(i)} - \boldsymbol{\alpha} \cdot \mathbf{A}^{(i)} - 2\beta) \}$$

on \mathcal{D}_N . For every $i \in \{1, \dots, N\}$, we further write

$$[\boldsymbol{\alpha} \cdot \mathbf{A}^{(i)}, F_\varepsilon^n] D_{\mathbf{A}}^{(i)} = Q_{\varepsilon,n}^{(i)} (D_{\mathbf{A}}^{(i)} F_\varepsilon^{n-1} - Q_{\varepsilon,n-1}^{(i)} F_\varepsilon^{n-2})$$

on \mathcal{D}_N , where

$$(4.11) \quad Q_{\varepsilon,n}^{(i)} := [\boldsymbol{\alpha} \cdot \mathbf{A}^{(i)}, F_\varepsilon^n] F_\varepsilon^{1-n}, \quad n \in \mathbb{N}, \quad Q_{\varepsilon,0}^{(i)} := 0.$$

According to (3.11) we have $\|Q_{\varepsilon,n}^{(i)}\| \leq n 2^{(n+2)/2} (d_1 + d_{3+n})$, $\|\check{H}_f^{1/2} Q_{\varepsilon,n}^{(i)} \check{H}_f^{-1/2}\| \leq n 2^{(n+3)/2} (d_1 + d_{4+n})$. Likewise, we write

$$[\boldsymbol{\alpha} \cdot \mathbf{A}^{(i)}, F_\varepsilon^n] \boldsymbol{\alpha} \cdot \mathbf{A}^{(i)} = Q_{\varepsilon,n}^{(i)} (\{\boldsymbol{\alpha} \cdot \mathbf{A}^{(i)} \check{H}_f^{-1/2}\} \check{H}_f^{1/2} F_\varepsilon^{n-1} - Q_{\varepsilon,n-1}^{(i)} F_\varepsilon^{n-2})$$

on \mathcal{D}_N , where $\|\boldsymbol{\alpha} \cdot \mathbf{A} \check{H}_f^{-1/2}\|^2 \leq 2d_0^2 + 4d_{-1}^2$ by (3.7). Furthermore, we observe that Lemma 3.2 is applicable to $\boldsymbol{\Sigma} \cdot \mathbf{B}$ as well instead of $\boldsymbol{\alpha} \cdot \mathbf{A}$; we simply have to replace the form factor \mathbf{G} by $\nabla_{\mathbf{x}} \wedge \mathbf{G}$ and to notice that $\|\boldsymbol{\Sigma} \cdot \mathbf{v}\|_{\mathcal{L}(\mathbb{C}^4)} = |\mathbf{v}|$, $\mathbf{v} \in \mathbb{R}^3$, in analogy to (3.6). Note that the indices of d_ℓ are shifted by 2 because of (4.6). Finally, we observe that Lemma 3.2 is applicable to $\nabla_{\mathbf{x}} \cdot \mathbf{A}$, too. To this end we have to replace \mathbf{G} by $(\nabla_{\mathbf{x}} \cdot \mathbf{G}, 0, 0)$ and d_ℓ by some universal constant times $d_{2+\ell}$ because of (4.7). Taking all these remarks into account we arrive at

$$\begin{aligned} |\langle \Psi_1 | [H'_{\text{nr}}, F_\varepsilon^n] \Psi_2 \rangle| &\leq \sum_{i=1}^N \left\{ \|\Psi_1\| \|[\boldsymbol{\Sigma} \cdot \mathbf{B}^{(i)}, F_\varepsilon^n] F_\varepsilon^{1-n}\| \|F_\varepsilon^{n-1} \Psi_2\| \right. \\ &+ \|\Psi_1\| \|[\text{div } \mathbf{A}^{(i)}, F_\varepsilon^n] F_\varepsilon^{1-n}\| \|F_\varepsilon^{n-1} \Psi_2\| \\ &+ \|\Psi_1\| \|\boldsymbol{\alpha} \cdot \mathbf{A} \check{H}_f^{-1/2}\| \|\check{H}_f^{1/2} Q_{\varepsilon,n}^{(i)} \check{H}_f^{-1/2}\| \|\check{H}_f^{1/2} F_\varepsilon^{n-1} \Psi_2\| \\ &+ \|\Psi_1\| \|Q_{\varepsilon,n}^{(i)}\| (2 \|D_{\mathbf{A}}^{(i)} F_\varepsilon^{n-1} \Psi_2\| + \|\boldsymbol{\alpha} \cdot \mathbf{A} \check{H}_f^{-1/2}\| \|\check{H}_f^{1/2} F_\varepsilon^{n-1} \Psi_2\|) \\ &\left. + 3 \|\Psi_1\| \|Q_{\varepsilon,n}^{(i)}\| \|Q_{\varepsilon,n-1}^{(i)}\| \|F_\varepsilon^{n-2} \Psi_2\| + 2 \|\Psi_1\| \|Q_{\varepsilon,n}^{(i)}\| \|\beta\| \|F_\varepsilon^{n-1} \Psi_2\| \right\}, \end{aligned}$$

for all $\Psi_1, \Psi_2 \in \mathcal{D}_N$. From this estimate, Lemma 3.2, and (4.5) we readily infer that Condition (c') is valid with $c_n = (|E_{\text{nr}}| + 1) C''(N, n, a, b, d_{-1}, \dots, d_{5+n})$. \square

5. THE SEMI-RELATIVISTIC PAULI-FIERZ OPERATOR

The semi-relativistic Pauli-Fierz operator is also acting in the Hilbert space \mathcal{H}_N introduced in (4.1). It is obtained by substituting the non-local operator $|D_{\mathbf{A}}|$ for $D_{\mathbf{A}}^2$ in H_{nr}^V . We thus define, a priori on the dense domain \mathcal{D}_N ,

$$H_{\text{sr}}^V \equiv H_{\text{sr}}^V(\mathbf{G}) := \sum_{i=1}^N |D_{\mathbf{A}}^{(i)}| + V + H_f,$$

where V is assumed to fulfill Hypothesis 4.1 with H_{nr}^0 replaced by H_{sr}^0 . To ensure that in the case of the Coulomb potential V_C defined in (4.4) this yields a well-defined self-adjoint operator we have to impose appropriate restrictions on the nuclear charges.

Example. In Proposition A.1 we show that $H_{\text{sr}}^{V_C}$ is semi-bounded below on \mathcal{D}_N provided that $Z_k \in (0, 2/\pi e^2]$, for all $k \in \{1, \dots, K\}$. Its proof is actually a straightforward consequence of (3.19) and a commutator estimate obtained in [10]. If all atomic numbers Z_k are strictly less than $2/\pi e^2$ we thus find $a \in (0, 1)$ and $b \in (0, \infty)$ such that

$$(5.1) \quad \sum_{i=1}^N \sum_{k=1}^K \frac{e^2 Z_k}{|\mathbf{x}_i - \mathbf{R}_k|} \leq a H_{\text{sr}}^0 + b$$

in the sense of quadratic forms on \mathcal{D}_N . In particular, V_C fulfills Hypothesis 4.1 with H_{nr}^0 replaced by H_{sr}^0 as long as $Z_k \in (0, 2/\pi e^2]$, for $k \in \{1, \dots, K\}$. \diamond

For potentials V as above H_{sr}^V has a self-adjoint Friedrichs extension which we denote again by the same symbol H_{sr}^V . Moreover, \mathcal{D}_N is a form core for H_{sr}^V and we have the following analogue of (4.5),

$$(5.2) \quad |D_{\mathbf{A}}^{(1)}|, \dots, |D_{\mathbf{A}}^{(N)}|, V_+, H_{\text{f}} \leq H_{\text{sr}}^{V_+} \leq (1 - a)^{-1} (H_{\text{sr}}^V + b)$$

on \mathcal{D}_N . In order to apply Corollary 2.3 to the semi-relativistic Pauli-Fierz operator we recall the following special case of [7, Corollary 3.7]:

LEMMA 5.1. *Assume that ω and \mathbf{G} fulfill Hypothesis 3.1. Let $\tau \in (0, 1]$. Then there exist $\delta > 0$ and $C \equiv C(\delta, \tau, d_1) \in (0, \infty)$ such that*

$$(5.3) \quad C + |D_{\mathbf{A}}| + \tau H_{\text{f}} \geq \delta (|D_{\mathbf{0}}| + H_{\text{f}}) \geq \delta (|D_{\mathbf{0}}| + \tau H_{\text{f}}) \geq \delta^2 |D_{\mathbf{A}}| - \delta C$$

in the sense of quadratic forms on \mathcal{D} .

In the next theorem we re-derive the higher order estimates obtained in [4] for the semi-relativistic Pauli-Fierz operator by means of Corollary 2.3. (The second estimate of Theorem 5.2 is actually slightly stronger than the corresponding one stated in [4].) The estimates of the following proof are also employed in Section 6 where we treat the no-pair operator. We set

$$E_{\text{sr}} := \inf \sigma[H_{\text{sr}}], \quad H'_{\text{sr}} := H_{\text{sr}}^V - E_{\text{sr}} + 1.$$

THEOREM 5.2. *Assume that ω and \mathbf{G} fulfill Hypothesis 3.1 and that V fulfills Hypothesis 4.1 with H_{nr}^0 replaced by H_{sr}^0 . Then, for every $m \in \mathbb{N}$, it follows that $\mathcal{D}((H_{\text{sr}}^V)^{m/2}) \subset \mathcal{D}(H_{\text{f}}^{m/2})$, $H_{\text{f}}^{m/2} (H'_{\text{sr}})^{-m/2}$ maps $\mathcal{D}(H_{\text{sr}}^V)$ into itself, and*

$$\begin{aligned} \| H_{\text{f}}^{m/2} (H'_{\text{sr}})^{-m/2} \| &\leq C(N, m, a, b, d_1, d_{3+m}) (|E_{\text{sr}}| + 1)^{(3m-2)/2}, \\ \| [H_{\text{f}}^{m/2}, H_{\text{sr}}^V] (H'_{\text{sr}})^{-m/2} \| &\leq C'(N, m, a, b, d_1, d_{3+m}) (|E_{\text{sr}}| + 1)^{(3m-1)/2}. \end{aligned}$$

Proof. Let $m \in \mathbb{N}$. We pick the function f_ε defined in (3.10) with $E = k_1 \vee C$. (k_1 is the constant appearing in Lemma 3.3 with $\kappa = m/2$, $\nu = 0$, and depends on m , d_1 , and d_{3+m} ; C is the one in (5.3).) We fix some $n \in \mathbb{N}$, $n \leq m$,

and verify Conditions (a), (b), and (c') of Theorem 2.1 and Corollary 2.2 with $F_\varepsilon = f_\varepsilon^{1/2}(H_f)$, $\varepsilon > 0$. The estimates (4.8) and (4.9) are still valid without any further change when the subscript nr is replaced by sr. Employing (5.3) twice and using (5.2) we obtain the following substitute of (4.10),

$$\begin{aligned} \langle F_\varepsilon \Psi \mid |D_{\mathbf{A}}| F_\varepsilon \Psi \rangle &\leq \delta^{-1} \| |D_{\mathbf{0}}|^{1/2} F_\varepsilon \Psi \|^2 + \delta^{-1} \| \check{H}_f^{1/2} F_\varepsilon \Psi \|^2 \\ &\leq \delta^{-1} \| f_\varepsilon \|_\infty (\| |D_{\mathbf{0}}|^{1/2} \Psi \|^2 + \| \check{H}_f^{1/2} \Psi \|^2) \leq C' \| f_\varepsilon \|_\infty \langle \Psi \mid H'_{\text{sr}} \Psi \rangle, \end{aligned}$$

for all $\Psi \in \mathcal{D}_N$. Altogether we see that Conditions (a) and (b) are satisfied. In order to verify (c') we set

$$(5.4) \quad U_{\varepsilon,n}^{(i)} := [S_{\mathbf{A}}^{(i)}, F_\varepsilon^n] F_\varepsilon^{1-n} = F_\varepsilon^n [F_\varepsilon^{-n}, S_{\mathbf{A}}^{(i)}] F_\varepsilon, \quad i \in \{1, \dots, N\}.$$

By virtue of (3.22) we know that the norms of $U_{\varepsilon,n}^{(i)}$ and $U_{\varepsilon,n}^{(i)} |D_{\mathbf{A}}^{(i)}|^{1/2}$ are bounded uniformly in $\varepsilon > 0$ by some constant, $C \in (0, \infty)$, that depends only on n, d_1 , and d_{3+n} . We employ the notation (4.11) and (5.4) to write

$$\begin{aligned} [H'_{\text{sr}}, F_\varepsilon^n] &= \sum_{i=1}^N [|D_{\mathbf{A}}^{(i)}|, F_\varepsilon^n] = \sum_{i=1}^N [S_{\mathbf{A}}^{(i)} D_{\mathbf{A}}^{(i)}, F_\varepsilon^n] \\ &= \sum_{i=1}^N \left\{ \{ U_{\varepsilon,n}^{(i)} |D_{\mathbf{A}}^{(i)}|^{1/2} \} S_{\mathbf{A}}^{(i)} |D_{\mathbf{A}}^{(i)}|^{1/2} F_\varepsilon^{n-1} \right. \\ &\quad \left. - U_{\varepsilon,n}^{(i)} Q_{\varepsilon,n-1}^{(i)} F_\varepsilon^{n-2} + S_{\mathbf{A}}^{(i)} Q_{\varepsilon,n}^{(i)} F_\varepsilon^{n-1} \right\}. \end{aligned}$$

The previous identity, (5.2), and $|D_{\mathbf{A}}| \geq 1$ permit to get

$$\begin{aligned} |\langle \Psi_1 \mid [H'_{\text{sr}}, F_\varepsilon^n] \Psi_2 \rangle| &\leq \sum_{i=1}^N \| \Psi_1 \| \{ C \| |D_{\mathbf{A}}^{(i)}|^{1/2} F_\varepsilon^{n-1} \Psi_2 \| \\ &\quad + C \| Q_{\varepsilon,n}^{(i)} \| \| F_\varepsilon^{n-2} \Psi_2 \| + \| Q_{\varepsilon,n}^{(i)} \| \| F_\varepsilon^{n-1} \Psi_2 \| \} \\ &\leq c_n \{ \| \Psi_1 \|^2 + \langle F_\varepsilon^{n-1} \Psi_2 \mid H'_{\text{sr}} F_\varepsilon^{n-1} \Psi_2 \rangle \}, \end{aligned}$$

for all $\Psi_1, \Psi_2 \in \mathcal{D}_N$ and some constant $c_n = C''(n, a, b, d_1, d_{3+n})(|E_{\text{sr}}| + 1)$. So (c') is fulfilled also and the assertion follows from Corollary 2.3. \square

6. THE NO-PAIR OPERATOR

We introduce the spectral projections

$$(6.1) \quad P_{\mathbf{A}}^+ := E_{[0,\infty)}(D_{\mathbf{A}}) = \frac{1}{2} \mathbb{1} + \frac{1}{2} S_{\mathbf{A}}, \quad P_{\mathbf{A}}^- := \mathbb{1} - P_{\mathbf{A}}^+.$$

The no-pair operator acts in the projected Hilbert space

$$\mathcal{H}_N^+ \equiv \mathcal{H}_N^+(\mathbf{G}) := P_{\mathbf{A},N}^+ \mathcal{H}_N, \quad P_{\mathbf{A},N}^+ := \prod_{i=1}^N P_{\mathbf{A}}^{+, (i)},$$

and is a priori defined on the dense domain $P_{\mathbf{A},N}^+ \mathcal{D}_N$ by

$$H_{\text{np}}^V \equiv H_{\text{np}}^V(\mathbf{G}) := P_{\mathbf{A},N}^+ \left\{ \sum_{i=1}^N D_{\mathbf{A}}^{(i)} + V + H_f \right\} P_{\mathbf{A},N}^+.$$

Notice that all operators $D_{\mathbf{A}}^{(1)}, \dots, D_{\mathbf{A}}^{(N)}$ and $P_{\mathbf{A}}^{+,(1)}, \dots, P_{\mathbf{A}}^{+,(N)}$ commute in pairs owing to the fact that the components of the vector potential $A^{(i)}(\mathbf{x})$, $A^{(j)}(\mathbf{y})$, $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$, $i, j \in \{1, 2, 3\}$, commute in the sense that all their spectral projections commute; see the appendix to [9] for more details. (Here we use the assumption that $\mathbf{G}_{\mathbf{x}}(-\mathbf{k}, \lambda) = \overline{\mathbf{G}_{\mathbf{x}}(\mathbf{k}, \lambda)}$.) So the order of the application of the projections $P_{\mathbf{A}}^{+,(i)}$ is immaterial. In this section we restrict the discussion to the case where V is given by the Coulomb potential V_C defined in (4.4). To have a handy notation we set

$$v_i := - \sum_{k=1}^K \frac{e^2 Z_k}{|\mathbf{x}_i - \mathbf{R}_k|}, \quad w_{ij} := \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|},$$

for all $i \in \{1, \dots, N\}$ and $1 \leq i < j \leq N$, respectively. Thanks to [10, Proof of Lemma 3.4(ii)], which implies that $P_{\mathbf{A}}^+$ maps \mathcal{D} into $\mathcal{D}(|D_0|) \cap \mathcal{D}(H_f^\nu)$, for every $\nu > 0$, and Hardy's inequality, we actually know that $H_{\text{np}}^{V_C}$ is well-defined on \mathcal{D}_N . In order to apply Corollary 2.3 to $H_{\text{np}}^{V_C}$ we extend $H_{\text{np}}^{V_C}$ to a continuously invertible operator on the whole space \mathcal{H}_N : We pick the complementary projection,

$$P_{\mathbf{A},N}^\perp := \mathbb{1} - P_{\mathbf{A},N}^+,$$

abbreviate

$$P_{\mathbf{A}}^{+,(i,j)} := P_{\mathbf{A}}^{+,(i)} P_{\mathbf{A}}^{+,(j)} = P_{\mathbf{A}}^{+,(j)} P_{\mathbf{A}}^{+,(i)}, \quad 1 \leq i < j \leq N,$$

and define the operator \tilde{H}_{np} a priori on the domain \mathcal{D}_N by

$$\begin{aligned} \tilde{H}_{\text{np}} &:= \sum_{i=1}^N \left\{ |D_{\mathbf{A}}^{(i)}| + P_{\mathbf{A}}^{+,(i)} v_i P_{\mathbf{A}}^{+,(i)} \right\} + \sum_{\substack{i,j=1 \\ i < j}}^N P_{\mathbf{A}}^{+,(i,j)} w_{ij} P_{\mathbf{A}}^{+,(i,j)} \\ (6.2) \quad &+ P_{\mathbf{A},N}^+ H_f P_{\mathbf{A},N}^+ + P_{\mathbf{A},N}^\perp H_f P_{\mathbf{A},N}^\perp. \end{aligned}$$

Evidently, we have $[\tilde{H}_{\text{np}}, P_{\mathbf{A},N}^+] = 0$ and $\tilde{H}_{\text{np}} P_{\mathbf{A},N}^+ = H_{\text{np}}^{V_C} P_{\mathbf{A},N}^+$ on \mathcal{D}_N . In Proposition A.2 we show that the quadratic forms of the no-pair operator $H_{\text{np}}^{V_C}$ and of \tilde{H}_{np} are semi-bounded below on \mathcal{D}_N provided that the atomic numbers $Z_1, \dots, Z_K \geq 0$ are less than the critical one of the Brown-Ravenhall model determined in [3],

$$(6.3) \quad Z_{\text{np}} := (2/e^2)/(2/\pi + \pi/2).$$

Therefore, both $H_{\text{np}}^{V_C}$ and \tilde{H}_{np} possess self-adjoint Friedrichs extensions which are again denoted by the same symbols in the sequel. \mathcal{D}_N is a form core for

\tilde{H}_{np} and we have the bound

$$(6.4) \quad \tilde{H}_{\text{np}} - \sum_{i=1}^N P_{\mathbf{A}}^{+, (i)} v_i P_{\mathbf{A}}^{+, (i)} \leq \frac{Z_{\text{np}} + |\mathcal{Z}|}{Z_{\text{np}} - |\mathcal{Z}|} (\tilde{H}_{\text{np}} + C(N, \mathcal{Z}, \mathcal{R}, d_{-1}, d_1, d_5))$$

on \mathcal{D}_N , where $|\mathcal{Z}| := \max\{Z_1, \dots, Z_K\} < Z_{\text{np}}$. Moreover, it makes sense to define

$$E_{\text{np}} := \inf \sigma[H_{\text{np}}^{\text{Vc}}],$$

so that

$$H'_{\text{np}} := \tilde{H}_{\text{np}} - E_{\text{np}} P_{\mathbf{A}, N}^+ + \mathbb{1} \geq \mathbb{1}.$$

THEOREM 6.1. *Assume that ω and \mathbf{G} fulfill Hypothesis 3.1 and let $N, K \in \mathbb{N}$, $e > 0$, $\mathcal{Z} = (Z_1, \dots, Z_K) \in [0, Z_{\text{np}})^K$, and $\mathcal{R} = \{\mathbf{R}_1, \dots, \mathbf{R}_K\} \subset \mathbb{R}^3$, where Z_{np} is defined in (6.3). Then $\mathcal{D}((H'_{\text{np}})^{m/2}) \subset \mathcal{D}(H_{\text{f}}^{m/2})$, for every $m \in \mathbb{N}$, and*

$$\begin{aligned} & \left\| H_{\text{f}}^{m/2} \upharpoonright_{\mathcal{H}_N^+} (H_{\text{np}} - (E_{\text{np}} - 1) \mathbb{1}_{\mathcal{H}_N^+})^{-m/2} \right\|_{\mathcal{L}(\mathcal{H}_N^+, \mathcal{H}_N)} \leq \left\| H_{\text{f}}^{m/2} (H'_{\text{np}})^{-m/2} \right\| \\ & \leq C(N, m, \mathcal{Z}, \mathcal{R}, e, d_{-1}, d_1, d_{5+m}) (1 + |E_{\text{np}}|)^{(3m-2)/2} < \infty. \end{aligned}$$

Proof. Let $m \in \mathbb{N}$. Again we pick the function f_ε defined in (3.10) and set $F_\varepsilon := f_\varepsilon^{1/2}(H_{\text{f}})$, $\varepsilon > 0$. This time we choose $E = \max\{k d_1^2, k_1, C\}$ where k is the constant appearing in (3.19), $C \equiv C(d_1)$ is the one in (5.3), and k_1 the one appearing in Lemma 3.3 with $|\kappa| = (m + 1)/2$, $|\nu| = 1/2$. Thus k_1 depends only on m, d_1 , and d_{5+m} . On account of Corollary 2.3 it suffices to show that the conditions (a)–(c) of Theorem 2.1 are fulfilled. To this end we observe that on \mathcal{D}_N the extended no-pair operator can be written as $H'_{\text{np}} = H_{\text{sr}}^0 + \mathbb{1} + W$, where

$$\begin{aligned} W := & \sum_{i=1}^N P_{\mathbf{A}}^{+, (i)} v_i P_{\mathbf{A}}^{+, (i)} + \sum_{\substack{i, j=1 \\ i < j}}^N P_{\mathbf{A}}^{+, (i, j)} w_{ij} P_{\mathbf{A}}^{+, (i, j)} \\ & - E_{\text{np}} P_{\mathbf{A}, N}^+ - 2\text{Re} [P_{\mathbf{A}, N}^+ H_{\text{f}} P_{\mathbf{A}, N}^\perp]. \end{aligned}$$

The semi-relativistic Pauli-Fierz operator H_{sr}^0 has already been treated in the previous section and the bound

$$(6.5) \quad H_{\text{f}} \leq 2P_{\mathbf{A}, N}^+ H_{\text{f}} P_{\mathbf{A}, N}^+ + 2P_{\mathbf{A}, N}^\perp H_{\text{f}} P_{\mathbf{A}, N}^\perp$$

together with (6.4) implies

$$(6.6) \quad H_{\text{sr}}^0 \leq 2\tilde{H}_{\text{np}} - 2\sum_{i=1}^N P_{\mathbf{A}}^{+, (i)} v_i P_{\mathbf{A}}^{+, (i)} \leq C'(1 + |E_{\text{np}}|) H'_{\text{np}}$$

on \mathcal{D}_N , for some $C' \equiv C'(N, \mathcal{Z}, \mathcal{R}, d_{-1}, d_1, d_5) \in (0, \infty)$. Hence, it only remains to consider the operator W .

We fix some $n \in \mathbb{N}$, $n \leq m$. When we verify (a) we can ignore the potentials v_i since they are negative. Using $[F_\varepsilon^n, P_{\mathbf{A},N}^\perp] = [P_{\mathbf{A},N}^+, F_\varepsilon^n]$ we obtain

$$\begin{aligned} & |2\operatorname{Re} \langle P_{\mathbf{A},N}^+ F_\varepsilon \Psi \mid H_f P_{\mathbf{A},N}^\perp F_\varepsilon \Psi \rangle| \\ & \leq \|H_f^{1/2} P_{\mathbf{A},N}^+ F_\varepsilon \Psi\|^2 + \|H_f^{1/2} P_{\mathbf{A},N}^\perp F_\varepsilon \Psi\|^2 \\ & \leq 2\|f_\varepsilon\|_\infty \|H_f^{1/2} P_{\mathbf{A},N}^+ \Psi\|^2 + 2\|f_\varepsilon\|_\infty \|H_f^{1/2} P_{\mathbf{A},N}^\perp \Psi\|^2 \\ & \quad + 4\|H_f^{1/2} [P_{\mathbf{A},N}^+, F_\varepsilon] \check{H}_f^{-1/2}\| \|\check{H}_f^{1/2} \Psi\|^2, \end{aligned}$$

for every $\Psi \in \mathcal{D}_N$, where, for all $n \in \mathbb{N}$ and $\nu \in \mathbb{R}$,

$$\begin{aligned} \check{H}_f^\nu [P_{\mathbf{A},N}^+, F_\varepsilon^n] \check{H}_f^{-\nu} F_\varepsilon^{1-n} &= \sum_{i=1}^N \left\{ \prod_{j=1}^{i-1} \check{H}_f^\nu P_{\mathbf{A}}^{+,(j)} \check{H}_f^{-\nu} \right\} \times \\ & \times \left\{ \check{H}_f^\nu [P_{\mathbf{A}}^{+,(i)}, F_\varepsilon^n] \check{H}_f^{-\nu} F_\varepsilon^{1-n} \right\} \left\{ \prod_{k=i+1}^N \check{H}_f^\nu F_\varepsilon^{n-1} P_{\mathbf{A}}^{+,(k)} \check{H}_f^{-\nu} F_\varepsilon^{1-n} \right\} \end{aligned}$$

on \mathcal{D}_N . On account of Corollary 3.4 we thus have, for $|\nu| \leq 1/2$,

$$(6.7) \quad \sup_{\varepsilon>0} \|H_f^\nu [P_{\mathbf{A},N}^+, F_\varepsilon^n] \check{H}_f^{-\nu} F_\varepsilon^{1-n}\| \leq C(N, n, d_1, d_{4+n}).$$

Likewise we have

$$(6.8) \quad \begin{aligned} & |\langle F_\varepsilon \Psi \mid P_{\mathbf{A}}^{+, (i,j)} w_{ij} P_{\mathbf{A}}^{+, (i,j)} F_\varepsilon \Psi \rangle| \leq 2\|f_\varepsilon\| \|w_{ij}^{1/2} P_{\mathbf{A}}^{+, (i,j)} \Psi\|^2 \\ & \quad + 4\|w_{ij}^{1/2} [P_{\mathbf{A}}^{+, (i,j)}, F_\varepsilon] \check{H}_f^{-1/2}\|^2 \|\check{H}_f^{1/2} \Psi\|^2, \end{aligned}$$

where the first norm in the second line of (6.8) is bounded (uniformly in $\varepsilon > 0$) due to Lemma 6.2. Taking these remarks, $v_i \leq 0$, (6.4), and (6.5) into account we infer that

$$\langle F_\varepsilon \Psi \mid H'_{\text{np}} F_\varepsilon \Psi \rangle \leq c_\varepsilon \langle \Psi \mid H'_{\text{np}} \Psi \rangle, \quad \Psi \in \mathcal{D}_N,$$

showing that (a) is fulfilled. The condition (b) with some constant $c^2 = C(N, \mathcal{L}, \mathcal{R}, d_{-1}, d_1, d_5)(1 + |E_{\text{np}}|)$ follows immediately from $F_\varepsilon^2 \leq \check{H}_f \leq H_{\text{sr}}^0 + E$ on \mathcal{D}_N and (6.6). Finally, we turn to Condition (c). To this end let $P_{\mathbf{A},N}^\sharp$ and $P_{\mathbf{A},N}^\flat$ be $P_{\mathbf{A},N}^+$ or $P_{\mathbf{A},N}^\perp$. On \mathcal{D}_N we clearly have

$$(6.9) \quad [P_{\mathbf{A},N}^\sharp H_f P_{\mathbf{A},N}^\flat, F_\varepsilon^n] = \pm [P_{\mathbf{A},N}^+, F_\varepsilon^n] H_f P_{\mathbf{A},N}^\flat \pm P_{\mathbf{A},N}^\sharp H_f [P_{\mathbf{A},N}^+, F_\varepsilon^n].$$

For $\Psi_1, \Psi_2 \in \mathcal{D}_N$, we thus obtain

$$(6.10) \quad \begin{aligned} & |\langle \Psi_1 \mid [P_{\mathbf{A},N}^\sharp H_f P_{\mathbf{A},N}^\flat, F_\varepsilon^n] \Psi_2 \rangle| \\ & \leq \|\check{H}_f^{1/2} \Psi_1\| \|\check{H}_f^{-1/2} [P_{\mathbf{A},N}^+, F_\varepsilon^n] H_f^{1/2} F_\varepsilon^{1-n}\| \|H_f^{1/2} F_\varepsilon^{n-1} P_{\mathbf{A},N}^\flat \Psi_2\| \\ & \quad + \|H_f^{1/2} P_{\mathbf{A},N}^\sharp \Psi_1\| \|H_f^{1/2} [P_{\mathbf{A},N}^+, F_\varepsilon^n] \check{H}_f^{-1/2} F_\varepsilon^{1-n}\| \|\check{H}_f^{1/2} F_\varepsilon^{n-1} \Psi_2\|, \end{aligned}$$

where we can further estimate

$$\begin{aligned}
 & \|H_f^{1/2} F_\varepsilon^{n-1} P_{\mathbf{A},N}^b \Psi_2\| \\
 & \leq \{1 + \|H_f^{1/2} F_\varepsilon^{n-1} P_{\mathbf{A},N}^+ \check{H}_f^{-1/2} F_\varepsilon^{1-n}\|\} \|\check{H}_f^{1/2} F_\varepsilon^{n-1} \Psi_2\| \\
 (6.11) \quad & \leq \{1 + \|H_f^{1/2} F_\varepsilon^{n-1} P_{\mathbf{A}}^+ \check{H}_f^{-1/2} F_\varepsilon^{1-n}\|^N\} \|\check{H}_f^{1/2} F_\varepsilon^{n-1} \Psi_2\|,
 \end{aligned}$$

and, of course,

$$(6.12) \quad \|\check{H}_f^{1/2} F_\varepsilon^{n-1} \Psi_2\| \leq \|\check{H}_f^{1/2} P_{\mathbf{A},N}^+ F_\varepsilon^{n-1} \Psi_2\| + \|\check{H}_f^{1/2} P_{\mathbf{A},N}^- F_\varepsilon^{n-1} \Psi_2\|.$$

The operator norms in (6.10) can be estimated by means of (6.7) with $\nu = \pm 1/2$, the one in the last line of (6.11) is bounded by some $C(n, d_1, d_{3+n}) \in (0, \infty)$ due to (3.21). In a similar fashion we obtain, for all $i, j \in \{1, \dots, N\}$, $i < j$, and $\Psi_1, \Psi_2 \in \mathcal{D}_N$,

$$\begin{aligned}
 & |\langle \Psi_1 | [P_{\mathbf{A}}^{+, (i,j)} w_{ij} P_{\mathbf{A}}^{+, (i,j)}, F_\varepsilon^n] \Psi_2 \rangle| \\
 & \leq \|F_\varepsilon^{1-n} w_{ij}^{1/2} [F_\varepsilon^n, P_{\mathbf{A}}^{+, (i,j)}] \check{H}_f^{-1/2}\| \|\check{H}_f^{1/2} \Psi_1\| \|F_\varepsilon^{n-1} w_{ij}^{1/2} P_{\mathbf{A}}^{+, (i,j)} \Psi_2\| \\
 (6.13) \quad & + \|w_{ij}^{1/2} P_{\mathbf{A}}^{+, (i,j)} \Psi_1\| \|w_{ij}^{1/2} [P_{\mathbf{A}}^{+, (i,j)}, F_\varepsilon^n] F_\varepsilon^{1-n} \check{H}_f^{-1/2}\| \|\check{H}_f^{1/2} F_\varepsilon^{n-1} \Psi_2\|.
 \end{aligned}$$

Here we can further estimate

$$\begin{aligned}
 & \|w_{ij}^{1/2} F_\varepsilon^{n-1} P_{\mathbf{A}}^{+, (i,j)} \Psi_2\| \leq \|w_{ij}^{1/2} P_{\mathbf{A}}^{+, (i,j)} F_\varepsilon^{n-1} \Psi_2\| \\
 (6.14) \quad & + \|w_{ij}^{1/2} [F_\varepsilon^{n-1}, P_{\mathbf{A}}^{+, (i,j)}] \check{H}_f^{-1/2} F_\varepsilon^{1-n}\| \|\check{H}_f^{1/2} F_\varepsilon^{n-1} \Psi_2\|.
 \end{aligned}$$

Lemma 6.2 below ensures that all operator norms in (6.13) and (6.14) that involve $w_{ij}^{1/2}$ are bounded uniformly in $\varepsilon > 0$ by constants depending only on e, n, d_1 , and d_{5+n} . Furthermore, it is now clear how to treat the terms involving v_i or E_{np} . (In order to treat v_i just replace $P_{\mathbf{A}}^{+, (i,j)}$ by $P_{\mathbf{A}}^{+, (i)}$, w_{ij} by v_i , and $w_{ij}^{1/2}$ by $|v_i|^{1/2}$ in (6.13) and (6.14).) Combining (6.9)–(6.14) and their analogues for the remaining operators in W we arrive at

$$\begin{aligned}
 & |\langle \Psi_1 | [W, F_\varepsilon^n] \Psi_2 \rangle| \\
 & \leq C \sum_{\# \in \{+, \pm\}} \{ \langle \Psi_1 | P_{\mathbf{A},N}^\# H_f P_{\mathbf{A},N}^\# \Psi_1 \rangle + \langle F_\varepsilon^{n-1} \Psi_2 | P_{\mathbf{A},N}^\# H_f P_{\mathbf{A},N}^\# F_\varepsilon^{n-1} \Psi_2 \rangle \} \\
 & + C \sum_{\substack{i,j=1 \\ i < j}}^N \{ \langle \Psi_1 | P_{\mathbf{A}}^{+, (i,j)} w_{ij} P_{\mathbf{A}}^{+, (i,j)} \Psi_1 \rangle \\
 & \quad + \langle F_\varepsilon^{n-1} \Psi_2 | P_{\mathbf{A}}^{+, (i,j)} w_{ij} P_{\mathbf{A}}^{+, (i,j)} F_\varepsilon^{n-1} \Psi_2 \rangle \} \\
 & + C \sum_{i=1}^N \{ \langle \Psi_1 | P_{\mathbf{A}}^{+, (i)} |v_i| P_{\mathbf{A}}^{+, (i)} \Psi_1 \rangle + \langle F_\varepsilon^{n-1} \Psi_2 | P_{\mathbf{A}}^{+, (i)} |v_i| P_{\mathbf{A}}^{+, (i)} F_\varepsilon^{n-1} \Psi_2 \rangle \} \\
 & + C (1 + |E_{\text{np}}|) \{ \|\Psi_1\|^2 + \|F_\varepsilon^{n-1} \Psi_2\|^2 \},
 \end{aligned}$$

for all $\Psi_1, \Psi_2 \in \mathcal{D}_N$ and some ε -independent $C \equiv C(N, n, e, d_1, d_{5+n}) \in (0, \infty)$. Employing successively (3.19), which implies $|v_i| \leq (\pi e^2 |\mathcal{Z}|/2) (|D_{\mathbf{A}}^{(i)}| + \check{H}_f)$,

after that (3.21), which yields $\|\check{H}_f^{1/2} P_{\mathbf{A}}^{+, (i)} \Psi\|^2 \leq C(d_1, d_4)(\|\check{H}_f^{1/2} P_{\mathbf{A}, N}^+ \Psi\|^2 + \|\check{H}_f^{1/2} P_{\mathbf{A}, N}^- \Psi\|^2)$, and finally (6.4) we conclude that Condition (c) is fulfilled with $c_n = C(N, n, \mathcal{Z}, \mathcal{R}, e, d_{-1}, d_1, d_{5+n})(1 + |E_{\text{np}}|)$. \square

LEMMA 6.2. *For all $i, j \in \{1, \dots, N\}$, $i < j$, $n \in \mathbb{Z}$, and $\sigma, \tau \geq 0$ with $\sigma + \tau \leq 1$,*

$$\begin{aligned} & \sup_{\varepsilon > 0} \|F_\varepsilon^{\sigma-n} w_{ij}^{1/2} [F_\varepsilon^n, P_{\mathbf{A}}^{+, (i, j)}] \check{H}_f^{-1/2} F_\varepsilon^\tau\| \\ &= \sup_{\varepsilon > 0} \|w_{ij}^{1/2} F_\varepsilon^\sigma [P_{\mathbf{A}}^{+, (i, j)}, F_\varepsilon^{-n}] \check{H}_f^{-1/2} F_\varepsilon^{n+\tau}\| \leq eC(n, d_1, d_{5+n}) < \infty. \end{aligned}$$

Proof. We write

$$w_{ij}^{1/2} F_\varepsilon^\sigma [P_{\mathbf{A}}^{+, (i)} P_{\mathbf{A}}^{+, (j)}, F_\varepsilon^{-n}] \check{H}_f^{-1/2} F_\varepsilon^{n+\tau} = Y_1 + w_{ij}^{1/2} Y_2 + Y_3,$$

where

$$\begin{aligned} Y_1 &:= \{w_{ij}^{1/2} F_\varepsilon^\sigma [P_{\mathbf{A}}^{+, (i)}, F_\varepsilon^{-n}] \check{H}_f^{-1/2} F_\varepsilon^{n+\tau}\} \{\check{H}_f^{1/2} F_\varepsilon^{-n-\tau} P_{\mathbf{A}}^{+, (j)} \check{H}_f^{-1/2} F_\varepsilon^{n+\tau}\}, \\ Y_2 &:= P_{\mathbf{A}}^{+, (i)} F_\varepsilon^\sigma [P_{\mathbf{A}}^{+, (j)}, F_\varepsilon^{-n}] \check{H}_f^{-1/2} F_\varepsilon^{n+\tau}, \\ Y_3 &:= w_{ij}^{1/2} [F_\varepsilon^\sigma, P_{\mathbf{A}}^{+, (i)}] [P_{\mathbf{A}}^{+, (j)}, F_\varepsilon^{-n}] \check{H}_f^{-1/2} F_\varepsilon^{n+\tau}. \end{aligned}$$

Applying Corollary 3.4 we immediately see that $\|Y_1\| \leq eC(n, d_1, d_{5+n})$ and that

$$\|Y_3\| \leq \|w_{ij}^{1/2} [F_\varepsilon^\sigma, P_{\mathbf{A}}^{+, (i)}] F_\varepsilon^{-\sigma}\| \|F_\varepsilon^\sigma [P_{\mathbf{A}}^{+, (j)}, F_\varepsilon^{-n}] F_\varepsilon^{n+\tau}\| \leq eC(n, d_1, d_{3+n})$$

uniformly in $\varepsilon > 0$. Employing (3.19) (with respect to the variable \mathbf{x}_j for each fixed \mathbf{x}_i) and using $\| |D_{\mathbf{A}}^{(j)}|^{1/2}, P_{\mathbf{A}}^{+, (i)} \| = 0$, we further get

$$\begin{aligned} & \|w_{ij}^{1/2} Y_2 \Psi\|^2 \\ & \leq (\pi e^2/2) \|P_{\mathbf{A}}^{+, (i)}\|^2 \| |D_{\mathbf{A}}^{(j)}|^{1/2} F_\varepsilon^\sigma [P_{\mathbf{A}}^{+, (j)}, F_\varepsilon^{-n}] F_\varepsilon^{n+\tau}\|^2 \|\check{H}_f^{-1/2}\|^2 \\ & \quad + (\pi e^2/2) \|\check{H}_f^{1/2} P_{\mathbf{A}}^{+, (i)} \check{H}_f^{-1/2}\|^2 \|\check{H}_f^{1/2} F_\varepsilon^\sigma [P_{\mathbf{A}}^{+, (i)}, F_\varepsilon^{-n}] \check{H}_f^{-1/2} F_\varepsilon^{n+\tau}\|^2. \end{aligned}$$

By Corollary 3.4 all norms on the right hand side are bounded uniformly in $\varepsilon > 0$ by constants depending only on n, d_1 , and d_{4+n} . \square

APPENDIX A. SEMI-BOUNDEDNESS OF $H_{\text{sr}}^{\text{VC}}$ AND $H_{\text{np}}^{\text{VC}}$

In this appendix we verify that the semi-relativistic Pauli-Fierz and no-pair operators with Coulomb potential are semi-bounded below for all nuclear charges less than the critical charges without radiation fields. We do not attempt to give good lower bounds on their spectra since this is not the topic addressed in this paper. Our aim here is essentially only to ensure that these operators possess self-adjoint Friedrichs extensions. We recall that the stability of matter of the second kind has been proven for the no-pair operator in [9] under certain restrictions on the fine-structure constant, the ultra-violet cut-off, and the nuclear charges. The stability of matter of the second kind is a much stronger property than mere semi-boundedness. It says that the operator is bounded below by some constant which is proportional to the total number of nuclei and electrons and uniform in the nuclear positions. The restrictions imposed

on the physical parameters in [9] do, however, not allow for all atomic numbers less than Z_{np} .

First, we consider the semi-relativistic Pauli-Fierz operator. The following proposition is a simple generalization of the bound (3.19) proven in [10] to the case of $N \in \mathbb{N}$ electrons and $K \in \mathbb{N}$ nuclei.

PROPOSITION A.1. *Assume that ω and \mathbf{G} fulfill Hypothesis 3.1 and let $N, K \in \mathbb{N}$, $e > 0$, $\mathcal{Z} = (Z_1, \dots, Z_K) \in (0, 2/\pi e^2]^K$, and $\mathcal{R} = \{\mathbf{R}_1, \dots, \mathbf{R}_K\} \subset \mathbb{R}^3$. Then*

$$(A.1) \quad \sum_{i=1}^N |D_{\mathbf{A}}^{(i)}| + V_{\mathbf{C}} + \delta H_{\text{f}} \geq -C(\delta, N, \mathcal{Z}, \mathcal{R}, d_1) > -\infty,$$

for every $\delta > 0$ in the sense of quadratic forms on \mathcal{D}_N .

Proof. In view of (3.19) we only have to explain how to localize the non-local kinetic energy terms. To begin with we recall the following bounds proven in [10, Lemmata 3.5 and 3.6]: For every $\chi \in C^\infty(\mathbb{R}_{\mathbf{x}}^3, [0, 1])$,

$$(A.2) \quad \|\chi, S_{\mathbf{A}}\| \leq \|\nabla\chi\|_\infty, \quad \|D_{\mathbf{A}}[\chi, [\chi, S_{\mathbf{A}}]]\| \leq 2\|\nabla\chi\|_\infty^2.$$

Now, let $\mathcal{B}_r(\mathbf{z})$ denote the open ball of radius $r > 0$ centered at $\mathbf{z} \in \mathbb{R}^3$ in \mathbb{R}^3 . We set $\varrho := \min\{|\mathbf{R}_k - \mathbf{R}_\ell| : k \neq \ell\}/2$ and pick a smooth partition of unity on \mathbb{R}^3 , $\{\chi_k\}_{k=0}^K$, such that $\chi_k \equiv 1$ on $\mathcal{B}_{\varrho/2}(\mathbf{R}_k)$ and $\text{supp}(\chi_k) \subset \mathcal{B}_\varrho(\mathbf{R}_k)$, for $k = 1, \dots, K$, and such that $\sum_{k=0}^K \chi_k^2 = 1$. Then we have the following IMS type localization formula,

$$(A.3) \quad |D_{\mathbf{A}}| = \sum_{k=0}^K \left\{ \chi_k |D_{\mathbf{A}}| \chi_k + \frac{1}{2} [\chi_k, [\chi_k, |D_{\mathbf{A}}|]] \right\}$$

on \mathcal{D} , for every $i \in \{1, \dots, N\}$. A direct calculation shows that

$$(A.4) \quad [\chi_k, [\chi_k, |D_{\mathbf{A}}|]] = 2i\boldsymbol{\alpha} \cdot (\nabla\chi_k) [\chi_k, S_{\mathbf{A}}] + D_{\mathbf{A}} [\chi_k, [\chi_k, S_{\mathbf{A}}]]$$

on \mathcal{D} . By virtue of (3.6) and (A.2) we thus get

$$(A.5) \quad \|\chi_k, [\chi_k, |D_{\mathbf{A}}|]\| \leq 4\|\nabla\chi\|_\infty^2,$$

for all $k \in \{0, \dots, K\}$. Since we are able to localize the kinetic energy terms and since, by the choice of the partition of unity, the functions $\mathbb{R}^3 \ni \mathbf{x} \mapsto |\mathbf{x} - \mathbf{R}_k|^{-1} \chi_\ell^2(\mathbf{x})$ are bounded, for $k \in \{1, \dots, K\}$, $\ell \in \{0, \dots, K\}$, $k \neq \ell$, the bound (A.1) is now an immediate consequence of (3.19) (with δ replaced by δ/N). (Here we also make use of the fact that the hypotheses on \mathbf{G} are translation invariant.) \square

Next, we turn to the no-pair operator discussed in Section 6. The semi-boundedness of the molecular N -electron no-pair operator is essentially a consequence of the following inequality [10, Equation (2.14)], valid for all ω and \mathbf{G} fulfilling Hypothesis 3.1, $\gamma \in (0, 2/(2/\pi + \pi/2))$, and $\delta > 0$,

$$(A.6) \quad P_{\mathbf{A}}^+ (D_{\mathbf{A}}^{(i)} - \gamma/|\mathbf{x}| + \delta H_{\text{f}}) P_{\mathbf{A}}^+ \geq P_{\mathbf{A}}^+ (c(\gamma) |D_{\mathbf{0}}| - C) P_{\mathbf{A}}^+,$$

in the sense of quadratic forms on $P_{\mathbf{A}}^+ \mathcal{D}$. Here $C \equiv C(\delta, \gamma, d_{-1}, d_0, d_1) \in (0, \infty)$ and $c(\gamma) \in (0, \infty)$ depends only on γ .

PROPOSITION A.2. *Assume that ω and \mathbf{G} fulfill Hypothesis 3.1 and let $N, K \in \mathbb{N}$, $e > 0$, $\mathcal{Z} = (Z_1, \dots, Z_K) \in (0, Z_{\text{np}})^K$, and $\mathcal{R} = \{\mathbf{R}_1, \dots, \mathbf{R}_K\} \subset \mathbb{R}^3$, where Z_{np} is defined in (6.3). Then the quadratic form associated with the operator \tilde{H}_{np} defined in (6.2) is semi-bounded below,*

$$\tilde{H}_{\text{np}} \geq -C(N, K, \mathcal{Z}, \mathcal{R}, d_{-1}, d_1, d_5) > -\infty,$$

in the sense of quadratic forms on \mathcal{D}_N .

Proof. We again employ the parameter $\varrho > 0$ and the partition of unity introduced in the paragraph succeeding (A.2). Thanks to [10, Proof of Lemma 3.4(ii)] we know that $P_{\mathbf{A}}^+$ maps $\mathcal{D}(D_{\mathbf{0}} \otimes H_f^\nu)$ into $\mathcal{D}(D_{\mathbf{0}} \otimes H_f^{\nu-1})$, for every $\nu \geq 1$. The IMS localization formula thus yields

$$\begin{aligned} & P_{\mathbf{A}}^{+, (i)} v_i P_{\mathbf{A}}^{+, (i)} \\ &= \sum_{k=0}^K \left\{ \chi_k^{(i)} P_{\mathbf{A}}^{+, (i)} v_i P_{\mathbf{A}}^{+, (i)} \chi_k^{(i)} + \frac{1}{2} [\chi_k^{(i)}, [\chi_k^{(i)}, P_{\mathbf{A}}^{+, (i)} v_i P_{\mathbf{A}}^{+, (i)}]] \right\} \end{aligned}$$

on $\mathcal{D}(D_{\mathbf{0}} \otimes H_f)$, where a superscript (i) indicates that $\chi_k = \chi_k^{(i)}$ depends on the variable \mathbf{x}_i . Using $v_i \leq 0$, we observe that

$$\begin{aligned} & [\chi_k^{(i)}, [\chi_k^{(i)}, P_{\mathbf{A}}^{+, (i)} v_i P_{\mathbf{A}}^{+, (i)}]] \\ &= -2 [\chi_k^{(i)}, P_{\mathbf{A}}^{+, (i)}] v_i [P_{\mathbf{A}}^{+, (i)}, \chi_k^{(i)}] \\ &\quad + 2 \operatorname{Re} \{ P_{\mathbf{A}}^{+, (i)} v_i [\chi_k^{(i)}, [\chi_k^{(i)}, P_{\mathbf{A}}^{+, (i)}]] \} \\ \text{(A.7)} \quad & \geq 2 \operatorname{Re} \{ P_{\mathbf{A}}^{+, (i)} v_i [\chi_k^{(i)}, [\chi_k^{(i)}, P_{\mathbf{A}}^{+, (i)}]] \}. \end{aligned}$$

We recall the following estimate proven in [10, Lemma 3.6], for every $\chi \in C^\infty(\mathbb{R}_{\mathbf{x}}^3, [0, 1])$,

$$\left\| \frac{1}{|\mathbf{x}|} [\chi, [\chi, P_{\mathbf{A}}^+]] \check{H}_f^{-1/2} \right\| \leq 8^{3/2} \|\nabla \chi\|_\infty^2,$$

where $\check{H}_f = H_f + E$ with $E \geq 1 \vee (4d_1)^2$. Together with (A.7) it implies

$$\begin{aligned} & \langle \Psi | [\chi_k^{(i)}, [\chi_k^{(i)}, P_{\mathbf{A}}^{+, (i)} v_i P_{\mathbf{A}}^{+, (i)}]] \Psi \rangle \\ & \geq -\delta \langle \Psi | \check{H}_f \Psi \rangle - (8^3 \|\nabla \chi_k\|_\infty^4 / \delta) \|\Psi\|^2, \end{aligned}$$

for all $k \in \{0, \dots, K\}$, $i \in \{1, \dots, N\}$, $\delta > 0$, and $\Psi \in \mathcal{D}(D_{\mathbf{0}} \otimes H_f)$. Next, we pick cut-off functions, $\zeta_1, \dots, \zeta_K \in C_0^\infty(\mathbb{R}_{\mathbf{x}}^3, [0, 1])$, such that $\zeta_k = 1$ in a neighborhood of \mathbf{R}_k and $\operatorname{supp}(\zeta_k) \subset \mathcal{B}_{\varrho/4}(\mathbf{R}_k)$, for $k \in \{1, \dots, K\}$. By construction, $\operatorname{supp}(\zeta_k) \cap \operatorname{supp}(\chi_\ell) = \emptyset$, for all $k \in \{1, \dots, K\}$ and $\ell \in \{0, \dots, K\}$ with $k \neq \ell$. Denoting $\bar{\zeta}_k := 1 - \zeta_k$ and using the superscript (i) to indicate that $\zeta_k = \zeta_k^{(i)}$

is a function of the variable \mathbf{x}_i , we obtain

$$\begin{aligned}
 & \langle \Psi | \chi_k^{(i)} P_{\mathbf{A}}^{+, (i)} v_i P_{\mathbf{A}}^{+, (i)} \chi_k^{(i)} \Psi \rangle \\
 &= - \left\langle \Psi \left| \chi_k^{(i)} P_{\mathbf{A}}^{+, (i)} \frac{e^2 Z_k}{|\mathbf{x}_i - \mathbf{R}_k|} P_{\mathbf{A}}^{+, (i)} \chi_k^{(i)} \Psi \right. \right\rangle \\
 (A.8) \quad & - \sum_{\substack{\ell=1 \\ \ell \neq k}}^K \left\langle \Psi \left| \chi_k^{(i)} P_{\mathbf{A}}^{+, (i)} \frac{e^2 Z_\ell \zeta_\ell^{(i)}}{|\mathbf{x}_i - \mathbf{R}_\ell|} P_{\mathbf{A}}^{+, (i)} \chi_k^{(i)} \Psi \right. \right\rangle
 \end{aligned}$$

$$(A.9) \quad - \sum_{\substack{\ell=1 \\ \ell \neq k}}^K \left\langle \Psi \left| \chi_k^{(i)} P_{\mathbf{A}}^{+, (i)} \frac{e^2 Z_\ell \bar{\zeta}_\ell^{(i)}}{|\mathbf{x}_i - \mathbf{R}_\ell|} P_{\mathbf{A}}^{+, (i)} \chi_k^{(i)} \Psi \right. \right\rangle,$$

for all $\Psi \in \mathcal{D}(D_0 \otimes H_f)$. The operators appearing in the scalar products in (A.9) are bounded by definition of $\bar{\zeta}_\ell$. Their norms depend only on \mathcal{R} since $e^2 Z_\ell < 1$. Furthermore, by virtue of Lemma A.3 below the term in (A.8) is bounded from below by $-\delta \langle \Psi | H_f \Psi \rangle - C_\delta \|\Psi\|^2$, for all $\delta > 0$ and some $C_\delta \equiv C_\delta(\mathcal{R}, d_1, d_4) \in (0, \infty)$; see (A.11).

Taking all the previous remarks into account, using (A.3)–(A.5), $w_{ij} \geq 0$, $|D_{\mathbf{A}}^{(i)}| \geq P_{\mathbf{A}}^{+, (i)} D_{\mathbf{A}}^{(i)} P_{\mathbf{A}}^{+, (i)}$, and writing

$$H_f = \frac{1}{N} \sum_{i=1}^N \sum_{k=0}^K \chi_k^{(i)} (P_{\mathbf{A}}^{+, (i)} + P_{\mathbf{A}}^{-, (i)}) H_f \chi_k^{(i)},$$

we deduce that

$$\begin{aligned}
 & \tilde{H}_{\text{np}} \\
 & \geq (1 - 3\delta) P_{\mathbf{A}, N}^+ H_f P_{\mathbf{A}, N}^+ + (1 - 3\delta) P_{\mathbf{A}, N}^\perp H_f P_{\mathbf{A}, N}^\perp \\
 & + \sum_{\sharp \in \{+, \perp\}} \sum_{k=0}^K P_{\mathbf{A}, N}^\sharp \left\{ \sum_{i=1}^N \chi_k^{(i)} P_{\mathbf{A}}^{+, (i)} \left(D_{\mathbf{A}}^{(i)} - \frac{e^2 Z_k}{|\mathbf{x}_i - \mathbf{R}_k|} + \frac{\delta}{N} H_f \right) P_{\mathbf{A}}^{+, (i)} \chi_k^{(i)} \right. \\
 & + \left. \frac{\delta}{N} \sum_{i=1}^N \left(\chi_k^{(i)} P_{\mathbf{A}}^{-, (i)} H_f P_{\mathbf{A}}^{-, (i)} \chi_k^{(i)} + \sum_{b=\pm} \chi_k^{(i)} P_{\mathbf{A}}^{b, (i)} [P_{\mathbf{A}}^{b, (i)}, H_f] \chi_k^{(i)} \right) \right\} P_{\mathbf{A}, N}^\sharp \\
 & - \text{const}(N, \mathcal{R}, d_1, d_4)
 \end{aligned}$$

on \mathcal{D}_N , for every $\delta > 0$. Thanks to Corollary 3.4 (with $\varepsilon = 0$) we know that $[P_{\mathbf{A}}^{b, (i)}, H_f] \check{H}_f^{-1/2}$ extends to an element of $\mathcal{L}(\mathcal{H}_N)$ whose norm is bounded by some constant depending only on d_1 and d_5 , whence

$$\begin{aligned}
 & \frac{\delta}{N} \sum_{i=1}^N \sum_{k=0}^K \langle \chi_k^{(i)} P_{\mathbf{A}, N}^\sharp \Psi | P_{\mathbf{A}}^{b, (i)} [P_{\mathbf{A}}^{b, (i)}, H_f] \chi_k^{(i)} P_{\mathbf{A}, N}^\sharp \Psi \rangle \\
 & \geq -(\delta/2) \|\check{H}_f^{-1/2} P_{\mathbf{A}, N}^\sharp \Psi\|^2 - (\delta/2) \|[P_{\mathbf{A}}^{b, (i)}, H_f] \check{H}_f^{-1/2}\|^2 \|\Psi\|^2,
 \end{aligned}$$

for every $\Psi \in \mathcal{D}_N$, $\sharp \in \{+, \perp\}$, and $b = \pm$. For a sufficiently small choice of $\delta > 0$, the assertion of the proposition now follows from the semi-boundedness

of $P_{\mathbf{A}}^{+, (i)}$ ($D_{\mathbf{A}}^{(i)} - e^2 Z_k / |\mathbf{x}_i - \mathbf{R}_k| + (\delta/N) H_f$) $P_{\mathbf{A}}^{+, (i)}$ ensured by (A.6) and the condition $Z_k < Z_{\text{np}}$. \square

LEMMA A.3. *Let $\zeta \in C_0^\infty(\mathbb{R}^3, [0, 1])$, $\chi \in C^\infty(\mathbb{R}^3, [0, 1])$, such that $0 \in \text{supp}(\zeta)$ and $\text{supp}(\zeta) \cap \text{supp}(\chi) = \emptyset$. Set $\check{H}_f := H_f + E$, where $E \geq k_1 \vee d_1^2$. Then*

$$(A.10) \quad \| D_{\mathbf{A}} H_f^{1/2} \zeta P_{\mathbf{A}}^+ \chi \check{H}_f^{-1/2} \| \leq C(\zeta, \chi, d_1, d_4),$$

$$(A.11) \quad \left\| \frac{\zeta}{|\mathbf{x}|} P_{\mathbf{A}}^+ \chi \check{H}_f^{-1/2} \right\| \leq C'(\zeta, \chi, d_1, d_4).$$

Proof. We pick some $\tilde{\chi} \in C^\infty(\mathbb{R}^3, [0, 1])$ such that $\text{supp}(\tilde{\chi}) \cap \text{supp}(\zeta) = \emptyset$ and $\tilde{\chi} \equiv 1$ on $\text{supp}(\nabla\chi)$. Using $\zeta \chi = 0 = \zeta \tilde{\chi}$ we infer that, for all $\varphi, \psi \in \mathcal{D}$,

$$\begin{aligned} |\langle D_{\mathbf{A}} \varphi | H_f^{1/2} \zeta P_{\mathbf{A}}^+ \chi \check{H}_f^{-1/2} \psi \rangle| &= |\langle D_{\mathbf{A}} \varphi | H_f^{1/2} \zeta [P_{\mathbf{A}}^+, \chi] \check{H}_f^{-1/2} \psi \rangle| \\ &\leq \int_{\mathbb{R}} \left| \langle D_{\mathbf{A}} \varphi | H_f^{1/2} \zeta [R_{\mathbf{A}}(iy), \tilde{\chi}] i\boldsymbol{\alpha} \cdot \nabla \chi R_{\mathbf{A}}(iy) \check{H}_f^{-1/2} \psi \rangle \right| \frac{dy}{2\pi} \\ &= \int_{\mathbb{R}} \left| \langle D_{\mathbf{A}} \varphi | H_f^{1/2} \zeta R_{\mathbf{A}}(iy) i\boldsymbol{\alpha} \cdot \nabla \tilde{\chi} R_{\mathbf{A}}(iy) i\boldsymbol{\alpha} \cdot \nabla \chi R_{\mathbf{A}}(iy) \check{H}_f^{-1/2} \psi \rangle \right| \frac{dy}{2\pi} \\ &= \int_{\mathbb{R}} \left| \langle \zeta D_{\mathbf{A}} \varphi | R_{\mathbf{A}}(iy) \Upsilon_{0,1/2}(iy) i\boldsymbol{\alpha} \cdot \nabla \tilde{\chi} R_{\mathbf{A}}(iy) \Upsilon_{0,1/2}(iy) \times \right. \\ &\quad \left. \times i\boldsymbol{\alpha} \cdot \nabla \chi R_{\mathbf{A}}(iy) \Upsilon_{0,1/2}(iy) \psi \rangle \right| \frac{dy}{2\pi}. \end{aligned}$$

In the last step we repeatedly applied (3.16). Commuting ζ and $D_{\mathbf{A}}$ and using $\|D_{\mathbf{A}} R_{\mathbf{A}}(iy)\| \leq 1$, $\|R_{\mathbf{A}}(iy)\|^2 \leq (1 + y^2)^{-1}$, and the fact that $\|\Upsilon_{0,1/2}(iy)\|$ is uniformly bounded in $y \in \mathbb{R}$, we readily deduce that

$$|\langle D_{\mathbf{A}} \varphi | H_f^{1/2} \zeta P_{\mathbf{A}}^+ \chi \check{H}_f^{-1/2} \psi \rangle| \leq C(\zeta, \chi, \tilde{\chi}, d_1, d_4) \|\varphi\| \|\psi\|,$$

which implies (A.10). The bound (A.11) follows from (A.10) and the inequality

$$\| |\mathbf{x}|^{-1} \varphi \|^2 \leq 4 \| D_{\mathbf{A}} \varphi \|^2 + 4 \| \check{H}_f^{1/2} \varphi \|^2, \quad \varphi \in \mathcal{D}(D_{\mathbf{0}} \otimes H_f^{1/2}),$$

which is a simple consequence of standard arguments (see, e.g., [10, Equation (4.7)]). \square

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