

GROUND STATES OF SEMI-RELATIVISTIC PAULI-FIERZ AND NO-PAIR HAMILTONIANS IN QED AT CRITICAL COULOMB COUPLING

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ABSTRACT. We consider the semi-relativistic Pauli–Fierz Hamiltonian and a no-pair model of a hydrogen-like atom interacting with a quantized photon field at the respective critical values of the Coulomb coupling constant. For arbitrary values of the fine-structure constant and the ultra-violet cutoff, we prove the existence of normalizable ground states of the atomic system in both models. This complements earlier results on the existence of ground states in (semi-)relativistic models of quantum electrodynamics at sub-critical coupling by E. Stockmeyer and the present authors. Technically, the main new achievement is an improved estimate on the spatial exponential localization of low-lying spectral subspaces yielding uniform bounds at large Coulomb coupling constants. In the semi-relativistic Pauli–Fierz model our exponential decay rate given in terms of the binding energy reduces to the one known from the electronic model when the radiation field is turned off. In particular, an increase of the binding energy due to the radiation field is shown to improve the localization of ground states.

KEYWORDS: *Existence of ground states, exponential localization, semi-relativistic Pauli–Fierz, no-pair Hamiltonian, quantum electrodynamics.*

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1. INTRODUCTION

By now the standard model non-relativistic quantum electrodynamics (QED) has been studied mathematically in great detail. In this model non-relativistic electrons described by molecular Schrödinger operators interact with a relativistic quantized photon field via minimal coupling. The resulting Hamiltonian is called the non-relativistic Pauli–Fierz (NRPF) operator. One may ask whether mathematical results on the NRPF operator can be extended to models accounting for the electrons by relativistic operators as well. There exist two such

models whose mathematical analysis seems canonical and interesting as an intermediate step towards full QED, where, besides the photon field, also electrons and positrons are described as quantized fields.

The first model is given by the *semi*-relativistic Pauli–Fierz (SRPF) operator where the non-relativistic kinetic energy of an electron in the NRPF model is replaced by its square root. This model has been treated mathematically for the first time in [26]. As mentioned by the authors in that paper the SRPF model can be formally derived by applying a canonical quantization procedure (described, e.g., in [32]) to a coupled system of differential equations comprised of the Maxwell equations with a rigid charge distribution and the evolution equation for a classical relativistic point particle. By choosing a static charge distribution — in our case the point charge of a nucleus located at the origin — one actually fixes a certain reference frame, which is one reason why the model is called semi-relativistic. As they are interested in electron dynamics the authors of [26] include spin. A scalar square-root Hamiltonian minimally coupled to the quantized radiation field appeared earlier in the mathematical analysis of Rayleigh scattering [8] which is related to the relaxation of excited states to an atomic ground state. In this situation the finite propagation speed of the electron is an advantageous feature of the dynamics generated by square root Hamiltonians.

The second model treated here is a no-pair model introduced in [20] in order to study the stability of relativistic matter interacting with the quantized radiation field. In this model the Schrödinger operators in the NRPF Hamiltonian are substituted by Dirac operators and the whole Hamiltonian is restricted to a subspace where all electrons live in positive spectral subspaces of free Dirac operators with minimally coupled vector potentials. The idea to employ no-pair models to describe atomic or molecular systems goes back to [3] and [33]. In the latter paper a no-pair Hamiltonian is formally derived starting from full QED by means of a procedure which neglects the creation and annihilation of electron-positron pairs — which explains the nomenclature. Nowadays, various no-pair models are extensively used, for instance, to include relativistic corrections in numerical computations in quantum chemistry; see, e.g., [30]. There is always a certain freedom in choosing the spectral subspaces determining a no-pair model. The conventions in [3], [33], for instance, force the electrons to live in positive spectral subspaces of a Dirac operator *without* magnetic vector potential. Investigations of the stability of relativistic matter revealed, however, that this choice — besides breaking gauge invariance — always leads to instability as soon as more than one electron is considered and the interaction with the ever present (classical or quantized) radiation field generated by the electrons is taken into account [11], [20], [22].

In the case of a hydrogen-like atom — that is, for one electron — both models mentioned above are introduced in detail in Section 3 after some notation has been fixed in Section 2. As already indicated they have both been investigated in

the mathematical literature before [8], [15], [19], [20], [26], but to a much lesser extent than models of non-relativistic QED. Their mathematical analysis is actually more difficult than in the non-relativistic case since the electronic and photonic degrees of freedom are coupled by *non-local* operators, namely the square roots and spectral projections of the Dirac operators, respectively. In our earlier works together with E. Stockmeyer [17], [18], [24] we gave some further contributions to these models by proving the existence of energy minimizing, exponentially localized ground states of the atomic system — a question which has been solved in non-relativistic QED in [1], [2], [9], [10], [21].

Typically, in relativistic atomic models there exist critical values, γ_c , of the Coulomb coupling constant, $\gamma \geq 0$, restricting the range where physically distinguished self-adjoint realizations of the Hamiltonian can be found. This is due to the fact that in relativistic Coulomb systems both the (positive) kinetic and the (negative) potential energy scale as one over the length. (In the physical application we have $\gamma = e^2 Z$, where e^2 is the square of the elementary charge and $Z \geq 0$ is the atomic number.) For the SRPF operator the critical value is equal to the critical constant in Kato's inequality, $2/\pi$. In the no-pair model the critical value is the one of the (purely electronic) Brown–Ravenhall operator, $2/(2/\pi + \pi/2)$ [6]. According to [17], [18] these critical values do not change when the interaction with the quantized photon field is taken into account. The main results of [17], [18] hold, however, only for sub-critical γ . In particular, the existence of ground states of hydrogen-like atoms at critical Coulomb coupling in the SRPF and no-pair models has not yet been proven and we wish to close this gap in the present article. We think that the analysis of the critical case is interesting for several reasons. First, the existence of an energy minimizing ground state of an atomic Hamiltonian which is kept fixed under the time evolution is a very fundamental notion in quantum theory. It is hence desirable to show that this conception holds true in our situation as soon as the definition of the Hamiltonian makes sense. Second, the mathematical investigation of the critical case is interesting in its own right as one cannot employ simple relative form bounds in order to control the Coulomb potential and has to make use of more refined estimates instead. Finally, by avoiding arguments requiring the Coulomb potential to be a small form perturbation we shall obtain estimates on the spatial exponential localization of low-energy states which are uniform in the Coulomb coupling constant and show that the decay rate of ground state eigenvectors increases as a function of the binding energy, as γ grows and approaches its critical value. This improves on earlier results on the localization of low-lying spectral subspaces of the SRPF and no-pair operators which provide only γ -dependent estimates [24]. In particular, we obtain a more realistic description of localization in our models, also for subcritical γ . In the SRPF model our new localization estimates can also be used to show that an increase of the binding energy due to the quantized radiation field (at fixed γ) leads to an improved localization of low-energy states. (In

fact, by simply ignoring the radiation field we can extend well-known exponential localization estimates in L^2 for the purely electronic square-root operator to all values of $\gamma \in [0, 2/\pi]$. In the literature we only found localization results for $\gamma \in (0, 1/2]$ [27].)

Presumably it is possible to directly prove the existence of ground states along the lines of [1], [10], [17], [18], also for $\gamma = \gamma_c$. We think, however, that it would be quite a tedious procedure to replace *all* arguments in [17], [18] that exploit the sub-criticality of γ by alternative ones. For instance, simple characterizations of the form domains of the Hamiltonians are available, for sub-critical γ , which is very convenient in order to argue that certain formal computations can be justified rigorously. Therefore, it seems more comfortable to pick some family of ground state eigenvectors, $\{\phi_\gamma\}_{\gamma < \gamma_c}$, and consider the limit $\gamma \nearrow \gamma_c$. To this end we shall apply a compactness argument in Section 5 similar to one used in [10] in order to remove an artificial photon mass. Among other ingredients this compactness argument requires the above-mentioned bound on the spatial localization of ϕ_γ , which is uniform for $\gamma \nearrow \gamma_c$. More precisely, we shall prove a suitable bound on the spatial exponential localization of spectral subspaces corresponding to energies below the ionization threshold which applies to all $\gamma \leq \gamma_c$. This localization estimate is derived in Section 4 by adapting and extending ideas from [1], [23], [24]. We remark that by now we are able to improve the localization estimates of [24] thanks to some more recent results of [18] collected in Proposition 3.3. At the end of Section 4 we discuss the electron Hamiltonians without radiation field and the improvement of localization in the SRPF model when the coupling to the radiation field is turned on. An important prerequisite for the analysis of both non-local models studied here are commutator estimates involving sign functions of Dirac operators, multiplication operators, and the radiation field energy. Many such estimates have been derived in [17], [18], [23], [24]. For our new proof of the exponential localization we need, however, still some additional ones. For this reason, and also to make this paper self-contained and the proofs comprehensible, we derive all required commutator estimates in Appendix A.

The main results of this paper are Theorem 4.5 (Exponential localization) and Theorem 5.4 (Existence of ground states at critical coupling).

2. NOTATION

The Hilbert space underlying the atomic models studied in this article is

$$(2.1) \quad \mathcal{H} := L^2(\mathbb{R}^3, \mathbb{C}^4) \otimes \mathcal{F}_b[\mathcal{K}] = \int_{\mathbb{R}^3}^{\oplus} \mathbb{C}^4 \otimes \mathcal{F}_b[\mathcal{K}] d^3\mathbf{x},$$

or a certain subspace of it. Here $\mathcal{F}_b[\mathcal{H}] = \bigoplus_{n=0}^{\infty} \mathcal{F}_b^{(n)}[\mathcal{H}]$ denotes the bosonic Fock space modeled over the one photon Hilbert space

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

The letter $k = (\mathbf{k}, \lambda)$ always denotes a tuple consisting of a photon wave vector, $\mathbf{k} \in \mathbb{R}^3$, and a polarization label, $\lambda \in \mathbb{Z}_2$. The components of \mathbf{k} are denoted as $\mathbf{k} = (k^{(1)}, k^{(2)}, k^{(3)})$. We recall that $\mathcal{F}_b^{(0)}[\mathcal{H}] := \mathbb{C}$ and, for $n \in \mathbb{N}$, $\mathcal{F}_b^{(n)}[\mathcal{H}] := \mathcal{S}_n L^2((\mathbb{R}^3 \times \mathbb{Z}_2)^n)$, where, for $\psi^{(n)} \in L^2((\mathbb{R}^3 \times \mathbb{Z}_2)^n)$,

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

\mathfrak{S}_n denoting the group of permutations of $\{1, \dots, n\}$. For $f \in \mathcal{H}$ and $n \in \mathbb{N}_0$, we further define $a^\dagger(f)^{(n)} : \mathcal{F}_b^{(n)}[\mathcal{H}] \rightarrow \mathcal{F}_b^{(n+1)}[\mathcal{H}]$ by $a^\dagger(f)^{(n)} \psi^{(n)} := \sqrt{n+1} \mathcal{S}_{n+1}(f \otimes \psi^{(n)})$. Then the standard bosonic creation operator is given by $a^\dagger(f) \psi := (0, a^\dagger(f)^{(0)} \psi^{(0)}, a^\dagger(f)^{(1)} \psi^{(1)}, \dots)$, for all $\psi = (\psi^{(0)}, \psi^{(1)}, \dots) \in \mathcal{F}_b[\mathcal{H}]$ such that the right side again belongs to $\mathcal{F}_b[\mathcal{H}]$. The corresponding annihilation operator is defined by $a(f) := a^\dagger(f)^*$ and we have the canonical commutation relations

$$(2.2) \quad [a^\sharp(f), a^\sharp(g)] = 0, \quad [a(f), a^\dagger(g)] = \langle f | g \rangle \mathbf{1}, \quad f, g \in \mathcal{H},$$

where a^\sharp is a^\dagger or a . Writing

$$(2.3) \quad \mathbf{k}_\perp := (k^{(2)}, -k^{(1)}, 0), \quad \mathbf{k} = (k^{(1)}, k^{(2)}, k^{(3)}) \in \mathbb{R}^3,$$

we introduce two polarization vectors,

$$(2.4) \quad \varepsilon(\mathbf{k}, 0) = \frac{\mathbf{k}_\perp}{|\mathbf{k}_\perp|}, \quad \varepsilon(\mathbf{k}, 1) = \frac{\mathbf{k}}{|\mathbf{k}|} \wedge \varepsilon(\mathbf{k}, 0),$$

for almost every $\mathbf{k} \in \mathbb{R}^3$. Moreover, we introduce a coupling function,

$$(2.5) \quad \mathbf{G}_x(k) = (G_x^{(1)}, G_x^{(2)}, G_x^{(3)})(k) := -e \frac{\mathbf{1}_{\{|\mathbf{k}| \leq \Lambda\}}}{2\pi |\mathbf{k}|^{1/2}} e^{-i\mathbf{k} \cdot \mathbf{x}} \varepsilon(k),$$

for all $\mathbf{x} \in \mathbb{R}^3$ and almost every $k = (\mathbf{k}, \lambda) \in \mathbb{R}^3 \times \mathbb{Z}_2$. The values of the ultraviolet cut-off, $\Lambda > 0$, and $e \in \mathbb{R}$ are arbitrary. (In the physical application e is the square root of Sommerfeld's fine structure constant and $e^2 \approx 1/137$.) For short, we write $a^\sharp(\mathbf{G}_x) := (a^\sharp(G_x^{(1)}), a^\sharp(G_x^{(2)}), a^\sharp(G_x^{(3)}))$. Then the quantized vector potential is the triple of operators $\mathbf{A} = (A^{(1)}, A^{(2)}, A^{(3)})$ in \mathcal{H} given as

$$(2.6) \quad \mathbf{A} := \int_{\mathbb{R}^3}^{\oplus} \mathbf{1}_{\mathbb{C}^4} \otimes (a^\dagger(\mathbf{G}_x) + a(\mathbf{G}_x)) d^3\mathbf{x}.$$

The radiation field energy is the second quantization, $H_f := d\Gamma(\omega)$, of the dispersion relation $\omega : \mathbb{R}^3 \times \mathbb{Z}_2 \rightarrow \mathbb{R}$, $k = (\mathbf{k}, \lambda) \mapsto \omega(k) := |\mathbf{k}|$. By definition, $d\Gamma(\omega)$

is the direct sum $d\Gamma(\omega) := \bigoplus_{n=0}^{\infty} d\Gamma^{(n)}(\omega)$, where $d\Gamma^{(0)}(\omega) := 0$, and $d\Gamma^{(n)}(\omega)$ is

the maximal multiplication operator in $\mathcal{F}_b^{(n)}[\mathcal{H}]$ associated with the symmetric function $(k_1, \dots, k_n) \mapsto \omega(k_1) + \dots + \omega(k_n)$, if $n \in \mathbb{N}$.

As usual we shall consider operators in $L^2(\mathbb{R}_x^3, \mathbb{C}^4)$ or $\mathcal{F}_b[\mathcal{H}]$ also as operators acting in the tensor product \mathcal{H} by identifying $|\hat{x}|^{-1} \equiv |\hat{x}|^{-1} \otimes \mathbf{1}$, $H_f \equiv \mathbf{1} \otimes H_f$, etc. (The hat $\hat{}$ indicates multiplication operators.)

Next, let $\alpha_0, \alpha_1, \alpha_2, \alpha_3$ denote hermitian 4×4 Dirac matrices obeying the Clifford algebra relations

$$(2.7) \quad \alpha_i \alpha_j + \alpha_j \alpha_i = 2 \delta_{ij} \mathbf{1}, \quad i, j \in \{0, 1, 2, 3\}.$$

In what follows they act on the second tensor factor in $\mathcal{H} = L^2(\mathbb{R}_x^3) \otimes \mathbb{C}^4 \otimes \mathcal{F}_b[\mathcal{H}]$. Then the free Dirac operator minimally coupled to \mathbf{A} is given as

$$(2.8) \quad D_{\mathbf{A}} := \boldsymbol{\alpha} \cdot (-i\nabla_x + \mathbf{A}) + \alpha_0 := \sum_{j=1}^3 \alpha_j (-i\partial_{x_j} + A^{(j)}) + \alpha_0.$$

It is clear that $D_{\mathbf{A}}$ is well-defined a priori on the dense domain

$$\mathcal{D} := C_0^\infty(\mathbb{R}^3, \mathbb{C}^4) \otimes \mathcal{C}, \quad (\text{algebraic tensor product})$$

where $\mathcal{C} \subset \mathcal{F}_b[\mathcal{H}]$ denotes the subspace of all $(\psi^{(n)})_{n=0}^\infty \in \mathcal{F}_b[\mathcal{H}]$ such that only finitely many components $\psi^{(n)}$ are non-zero and such that each $\psi^{(n)}$, $n \in \mathbb{N}$, is essentially bounded with compact support. Moreover, it is well-known that $D_{\mathbf{A}}$ is essentially self-adjoint on \mathcal{D} ; see, e.g., [20]. We use the symbol $D_{\mathbf{A}}$ again to denote its closure starting from \mathcal{D} .

Finally, we use the symbols $\mathcal{D}(T)$ and $\mathcal{Q}(T)$ to denote the domain and form domain, respectively, of some suitable operator T . We put $a \wedge b := \min\{a, b\}$, $a \vee b := \max\{a, b\}$, $a, b \in \mathbb{R}$, and $\langle y \rangle := (1 + y^2)^{1/2}$, $y \in \mathbb{R}$. $C(a, b, \dots)$, $C'(a, b, \dots)$, \dots denote positive constants which depend only on the quantities a, b, \dots displayed in their arguments and whose values might change from one estimate to another.

3. THE SEMI-RELATIVISTIC PAULI-FIERZ AND NO-PAIR MODELS

In what follows we shall denote the maximal operator of multiplication with the Coulomb potential, $-\gamma/|\mathbf{x}|$, $\gamma \geq 0$, in \mathcal{H} by V_γ . Then the semi-relativistic Pauli-Fierz (SRPF) operator is defined, a priori on the dense domain \mathcal{D} , as

$$H_\gamma^{\text{sr}} := |D_{\mathbf{A}}| + V_\gamma + H_f.$$

Notice that the absolute value $|D_{\mathbf{A}}|$ is actually a square root operator minimally coupled to \mathbf{A} . For, if the Dirac matrices are given in the standard representation, then

$$|D_{\mathbf{A}}| = \mathcal{T}_{\mathbf{A}}^{1/2} \oplus \mathcal{T}_{\mathbf{A}}^{1/2}, \quad \mathcal{T}_{\mathbf{A}} := (\boldsymbol{\sigma} \cdot (-i\nabla_x + \mathbf{A}))^2 + \mathbf{1},$$

where σ is a formal vector containing the three 2×2 Pauli spin matrices. According to [18] the quadratic form associated with H_γ^{sr} is semi-bounded below, if and only if γ is less than or equal to the critical constant in Kato's inequality,

$$\gamma_c^{\text{sr}} := \frac{2}{\pi}.$$

Thus, the range of stability of H_γ^{sr} is the same as the one of the purely electronic square root, or, Herbst [14] operator,

$$(3.1) \quad H_\gamma^{\text{el, sr}} := \sqrt{1 - \Delta_{\mathbf{x}}} + V_\gamma.$$

From now on the symbol H_γ^{sr} will again denote the Friedrichs extension of the SRPF operator, provided that $\gamma \in [0, \gamma_c^{\text{sr}}]$.

Compared to the non-relativistic Pauli–Fierz model there are only a few mathematical works dealing with its semi-relativistic analogue: Spinless square root operators coupled to quantized fields appear in the study of Rayleigh scattering in [8] and the fiber decomposition of $H_{\gamma=0}^{\text{sr}}$ is investigated in [26]. To recall some further results we define the ionization threshold and the ground state energy of H_γ^{sr} , respectively, as

$$\Sigma^{\text{sr}} := \inf \sigma[H_0^{\text{sr}}], \quad E_\gamma^{\text{sr}} := \inf \sigma[H_\gamma^{\text{sr}}], \quad \gamma \in (0, \gamma_c^{\text{sr}}).$$

Then the following shall be relevant for us:

PROPOSITION 3.1 ([15], [17]). (i) For all $e \in \mathbb{R}$, $\Lambda > 0$, and $\gamma \in (0, \gamma_c^{\text{sr}}]$,

$$(3.2) \quad \Sigma^{\text{sr}} - E_\gamma^{\text{sr}} \geq 1 - \inf \sigma[H_\gamma^{\text{el, sr}}] > 0.$$

(ii) For all $e \in \mathbb{R}$, $\Lambda > 0$, and $\gamma \in (0, \gamma_c^{\text{sr}})$, E_γ^{sr} is an eigenvalue of H_γ^{sr} .

Proof. Part (i) follows from [15] (at least in the case $\gamma \in (0, 1/2)$, where H_γ^{sr} is essentially self-adjoint on \mathcal{D} [18]). An alternative proof of (3.2) covering all $\gamma \in (0, \gamma_c^{\text{sr}}]$ can be found in [17]. Part (ii) is the main result of [17]. ■

In the present paper we shall extend the results on the spatial exponential localization of spectral subspaces below Σ^{sr} of H_γ^{sr} , $\gamma \in (0, \gamma_c^{\text{sr}})$, [24] and Proposition 3.1(ii) to the critical case $\gamma = \gamma_c^{\text{sr}}$.

In order to introduce the second model studied in this paper we first recall that the spectrum of $D_{\mathbf{A}}$ consists of two half-lines, $\sigma(D_{\mathbf{A}}) = (-\infty, -1] \cup [1, \infty)$. We denote the orthogonal projections onto the positive and negative spectral subspaces by

$$P_{\mathbf{A}}^\pm := \mathbf{1}_{\mathbb{R}^\pm}(D_{\mathbf{A}}) = \frac{1}{2} \mathbf{1} \pm \frac{1}{2} S_{\mathbf{A}}, \quad S_{\mathbf{A}} := D_{\mathbf{A}} |D_{\mathbf{A}}|^{-1}.$$

Then the no-pair operator is a self-adjoint operator acting in the positive spectral subspace $P_{\mathbf{A}}^+ \mathcal{H}$ defined, a priori on the dense domain $P_{\mathbf{A}}^+ \mathcal{D} \subset P_{\mathbf{A}}^+ \mathcal{H}$, by

$$(3.3) \quad H_\gamma^+ := P_{\mathbf{A}}^+ (D_{\mathbf{A}} + V_\gamma + H_f) P_{\mathbf{A}}^+.$$

Thanks to proof of Lemma 3.4(ii) of [24], which implies that $P_{\mathbf{A}}^+$ maps the subspace \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_γ^+ is well-defined on \mathcal{D} . Due to [18] the quadratic form associated with H_γ^+ is semi-bounded below, if and only if γ is less than or equal to

$$\gamma_c^{\text{np}} := \frac{2}{2/\pi + \pi/2},$$

which is the critical constant for the stability of the electronic Brown–Ravenhall operator,

$$(3.4) \quad H_\gamma^{\text{el,np}} := P_0^+ (D_0 + V_\gamma) P_0^+.$$

The value of γ_c^{np} has been determined in [6]. Again we denote the Friedrichs extension of the no-pair operator by the same symbol H_γ^+ , if $\gamma \in [0, \gamma_c^{\text{np}}]$. Because of technical reasons it is convenient to add the following counter-part acting in the negative spectral subspace $P_{\mathbf{A}}^- \mathcal{H}$,

$$H_\gamma^- := P_{\mathbf{A}}^- (-D_{\mathbf{A}} + V_\gamma + H_f) P_{\mathbf{A}}^-, \quad \gamma \in [0, \gamma_c^{\text{np}}],$$

which is also defined as a Friedrichs extension starting from \mathcal{D} . In fact, H_γ^+ and H_γ^- are unitarily equivalent as the unitary and symmetric matrix $\vartheta := \alpha_1 \alpha_2 \alpha_3 \alpha_0$ anti-commutes with $D_{\mathbf{A}}$, so that $\vartheta P_{\mathbf{A}}^+ = P_{\mathbf{A}}^- \vartheta$. Thus, if questions like localization and existence of ground states are addressed, then we may equally well consider the operator

$$(3.5) \quad H_\gamma^{\text{np}} := H_\gamma^+ \oplus H_\gamma^- = H_\gamma^+ \oplus \{\vartheta H_\gamma^+ \vartheta\}.$$

For later reference we observe that

$$(3.6) \quad H_\gamma^{\text{np}} = |D_{\mathbf{A}}| + \frac{1}{2} (V_\gamma + H_f) + \frac{1}{2} S_{\mathbf{A}} (V_\gamma + H_f) S_{\mathbf{A}} \quad \text{on } \mathcal{D}.$$

The mathematical analysis of a molecular analogue of H_γ^+ has been initiated in [20] where the stability of the second kind of relativistic matter has been established in the no-pair model under certain restrictions on e , Λ , and the nuclear charges. Moreover, an upper bound on the (positive) binding energy is derived in [19]. To recall some results on hydrogen-like atoms used later on we put

$$\Sigma^{\text{np}} := \inf \sigma[H_0^{\text{np}}], \quad E_\gamma^{\text{np}} := \inf \sigma[H_\gamma^{\text{np}}], \quad \gamma \in (0, \gamma_c^{\text{np}}].$$

Both parts of the following proposition are proven in [18]:

PROPOSITION 3.2 ([18]). (i) For all $e \in \mathbb{R}$, $\Lambda > 0$, and $\gamma \in (0, \gamma_c^{\text{np}}]$, there is some $c(\gamma, e, \Lambda) > 0$ such that

$$(3.7) \quad \Sigma^{\text{np}} - E_\gamma^{\text{np}} \geq c(\gamma, e, \Lambda).$$

(ii) For all $e \in \mathbb{R}$, $\Lambda > 0$, and $\gamma \in (0, \gamma_c^{\text{np}})$, E_γ^{np} is an eigenvalue of H_γ^{np} .

The exponential localization of spectral subspaces corresponding to energies below Σ^{np} is shown in [24], again for sub-critical values of γ only. We propose to extend the latter result as well as Proposition 3.2(ii) to the case $\gamma = \gamma_c^{\text{np}}$ in the present article.

We close this section by recalling some further results of [18] used later on. In order to improve the localization estimates of [24] and to deal with critical coupling constants the bounds in (3.8) below are particularly important. For they allow to control small pieces of the electronic kinetic energy by the total Hamiltonian even in the critical cases. Their proofs involve a strengthened version of the sharp generalized Hardy inequality obtained recently in [7], [31] and an analogous inequality for the Brown–Ravenhall model [7].

PROPOSITION 3.3 ([18]). *Let γ_c be γ_c^{sr} or γ_c^{np} and H_γ be H_γ^{sr} or H_γ^{np} . Then, for all $e \in \mathbb{R}$ and $\Lambda > 0$, the following holds:*

- (i) *For $\gamma \in [0, 1/2)$, H_γ is essentially self-adjoint on \mathcal{D} .*
- (ii) *For all $\varepsilon \in (0, 1)$, $\delta > 0$, and $\gamma \in [0, \gamma_c]$,*

$$(3.8) \quad |D_0|^\varepsilon \leq \delta H_\gamma + C(e, \Lambda, \delta, \varepsilon), \quad |D_A|^\varepsilon \leq \delta H_\gamma + C'(e, \Lambda, \delta, \varepsilon),$$

in the sense of quadratic forms on $\mathcal{Q}(H_\gamma)$.

- (iii) *$\mathcal{D}(H_\gamma) \subset \mathcal{D}(H_f)$ and, for all $\delta > 0$, $\gamma \in [0, \gamma_c]$, and $\psi \in \mathcal{D}(H_\gamma)$,*

$$(3.9) \quad \|H_f \psi\| \leq (1 + \delta) \|H_\gamma \psi\| + C(e, \Lambda, \delta) \|\psi\|.$$

4. EXPONENTIAL LOCALIZATION

In this section we show that low-lying spectral subspaces of H_γ^{sr} and H_γ^{np} are exponentially localized with respect to \mathbf{x} in a L^2 sense. This result is stated and proven in Theorem 4.5 later on. The general idea behind its proof, which rests on a simple identity involving the spectral projection (see (4.9)) and the Helffer–Sjöstrand formula, is due to [1]. (More precisely, (4.9) is variant of a similar identity used in [1]. It has been employed earlier in [23].) From a technical point of view the key step in the proof consists, however, in showing that the resolvent of a certain comparison operator stays bounded after the conjugation with exponential weights (Lemma 4.4). Moreover, one has to derive a useful resolvent identity involving the comparison operator and the original one (Lemma 4.2). In these steps our arguments are more streamlined and simpler than those used in the earlier paper [24] as we work with a simpler comparison operator. Moreover, we now treat critical γ as well. By now these improvements are possible thanks to the results of [18] collected in Proposition 3.3.

In the whole section we fix some $\mu \in C_0^\infty(\mathbb{R}_x^3, [0, 1])$ such that $\mu = 1$ on $\{|\mathbf{x}| \leq 1\}$ and $\mu = 0$ on $\{|\mathbf{x}| \geq 2\}$ and set $\mu_R(\mathbf{x}) := \mu(\mathbf{x}/R)$, for all $\mathbf{x} \in \mathbb{R}^3$ and

$R \geq 1$. Then we put

$$V_{\gamma,R} := (1 - \mu_R) V_\gamma = (\mu_R - 1) \frac{\gamma}{|\widehat{\mathbf{x}}|},$$

and define two comparison operators (compare (3.6)),

$$\begin{aligned} H_{\gamma,R}^{\text{sr}} &:= |D_{\mathbf{A}}| + V_{\gamma,R} + H_f, \quad \gamma \in (0, \gamma_c^{\text{sr}}], \\ H_{\gamma,R}^{\text{np}} &:= |D_{\mathbf{A}}| + \frac{1}{2} (V_{\gamma,R} + H_f) + \frac{1}{2} S_{\mathbf{A}} (V_{\gamma,R} + H_f) S_{\mathbf{A}}, \quad \gamma \in (0, \gamma_c^{\text{np}}], \end{aligned}$$

on the domain \mathcal{D} to start with. According to Proposition 3.3(i) both operators then are essentially self-adjoint and we again use the symbols $H_{\gamma,R}^{\text{sr}}$ and $H_{\gamma,R}^{\text{np}}$ to denote their self-adjoint closures. Clearly,

$$(4.1) \quad H_{\gamma,R}^{\text{sr}} \geq \Sigma^{\text{sr}} - \|V_{\gamma,R}\|_\infty, \quad H_{\gamma,R}^{\text{np}} \geq \Sigma^{\text{np}} - \|V_{\gamma,R}\|_\infty,$$

where $\|V_{\gamma,R}\|_\infty \leq 1/R$, $R \geq 1$. In order to treat both models at the same time we shall use the following notation from now on:

$$(4.2) \quad \begin{cases} \text{The symbols } H, H_R, \Sigma, E \text{ denote either} \\ H_\gamma^{\text{sr}}, H_{\gamma,R}^{\text{sr}}, \Sigma^{\text{sr}}, E_\gamma^{\text{sr}} \text{ or } H_\gamma^{\text{np}}, H_{\gamma,R}^{\text{np}}, \Sigma^{\text{np}}, E_\gamma^{\text{np}}. \end{cases}$$

Since the domains of H and H_R will in general be different we cannot compare their resolvents by means of the second resolvent identity. To overcome this problem we shall regularize the difference of their resolvents by means of the following cut-off function, which is also kept fixed throughout the whole section:

We pick some $\chi \in C^\infty(\mathbb{R}_{\mathbf{x}}^3, [0, 1])$ such that $\chi = 0$ on $\{|\mathbf{x}| \leq 2\}$ and $\chi = 1$ on $\{|\mathbf{x}| \geq 4\}$ and set $\chi_R(\mathbf{x}) := \chi(\mathbf{x}/R)$, for all $\mathbf{x} \in \mathbb{R}^3$ and $R \geq 1$.

Finally, we introduce a class of weight functions,

$$\mathcal{W}_a := \{F \in C^\infty(\mathbb{R}_{\mathbf{x}}^3, [0, \infty)) : F(\mathbf{0}) = 0, \|F\|_\infty < \infty, |\nabla F| \leq a\},$$

where $a \in (0, 1)$, and define two families of operators on the dense domain \mathcal{D} ,

$$U_R^F(z) := (H - z)^{-1} (H_R - H) \chi_R e^F, \quad W_R^F(z) := (H - z)^{-1} [\chi_R, H_R] e^F,$$

for $z \in \mathbb{C} \setminus \mathbb{R}$, $R \geq 1$, $F \in \mathcal{W}_a$, and $a \in (0, 1)$. Since $(V_\gamma - V_{\gamma,R}) \chi_R = 0$ we actually have $U_R^F(z) = 0$ when $H = H_\gamma^{\text{sr}}$.

In the whole section the positive constants $C(a, e, \dots)$, $C'(a, \dots)$, \dots are increasing functions of each displayed parameter when the others are kept fixed.

LEMMA 4.1. *Let $z \in \mathbb{C} \setminus \mathbb{R}$, $R \geq 1$, $F \in \mathcal{W}_a$, and $a \in (0, 1)$. Then $U_R^F(z)$ and $W_R^F(z)$ extend to bounded operators on \mathcal{H} and*

$$\sup_{F \in \mathcal{W}_a} \|U_R^F(z)\| + \sup_{F \in \mathcal{W}_a} \|W_R^F(z)\| \leq C(a, e, \Lambda, R) \frac{1 \vee |\operatorname{Re} z|}{1 \wedge |\operatorname{Im} z|}.$$

Proof. In the case of the no-pair operator we have

$$U_R^F(z) = \frac{1}{2} S_{\mathbf{A}} (H_\gamma^{\text{np}} - z)^{-1} (V_{\gamma,R} - V_\gamma) e^F [e^{-F} S_{\mathbf{A}} e^F, \chi_R] \quad \text{on } \mathcal{D},$$

where we used $[H_\gamma^{\text{np}}, S_{\mathbf{A}}] = 0 = (V_\gamma - V_{\gamma,R}) \chi_R$. In Lemma A.2 we shall show that

$$\| |\widehat{\chi}|^{-\kappa} (H_f + 1)^{-1/2} [e^{-F} S_{\mathbf{A}} e^F, \chi_R] \| \leq C(a, e, \Lambda, \kappa) \frac{\|\nabla \chi\|}{R},$$

for every $\kappa \in [0, 1)$. Combining the previous bound with the following consequence of $|\widehat{\chi}|^{-1/2} \leq C |D_0|^{1/2}$, (3.8), and (3.9),

$$\| |\widehat{\chi}|^{-1/8} H_f^{1/2} \psi \|^2 \leq \| |\widehat{\chi}|^{-1/4} \psi \| \| H_f \psi \| \leq C(e, \Lambda) \frac{1 \vee |\operatorname{Re} z|^2}{1 \wedge |\operatorname{Im} z|^2} \|(H_\gamma^{\text{np}} - \bar{z}) \psi\|^2,$$

for every $\psi \in \mathcal{D}(H_\gamma^{\text{np}})$, we deduce that

$$\begin{aligned} \| U_R^F(z) \varphi \| &\leq \frac{1}{2} \| |\widehat{\chi}|^{-1/8} (H_f + 1)^{1/2} (H_\gamma^{\text{np}} - \bar{z})^{-1} \| \| e^F \mu_R \| \\ &\quad \cdot \| |\widehat{\chi}|^{-7/8} (H_f + 1)^{-1/2} [e^{-F} S_{\mathbf{A}} e^F, \chi_R] \varphi \| \\ &\leq C'(a, e, \Lambda) \frac{e^{2aR}}{R} \frac{1 \vee |\operatorname{Re} z|}{1 \wedge |\operatorname{Im} z|} \| \varphi \|, \quad \varphi \in \mathcal{D}. \end{aligned}$$

Next, we turn to $W_R^F(z)$. In the case of the SRPF operator we have $[\chi_R, H_{\gamma,R}^{\text{sr}}] = [\chi_R, |D_{\mathbf{A}}|]$, and it follows from Lemma A.3 that, for all $F \in \mathcal{W}_a$,

$$(4.3) \quad \| [\chi_R, S_{\mathbf{A}}] e^F \| + \| |D_{\mathbf{A}}|^{-1/4} [\chi_R, |D_{\mathbf{A}}|] e^F \| \leq C(a) \| \nabla \chi_R e^F \|_\infty \leq C'(a, R).$$

Here we also used that $0 \leq F \leq 4aR$ on $\operatorname{supp}(\nabla \chi_R)$. On account of (3.8) we also have

$$\| |D_{\mathbf{A}}|^{1/4} (H_\gamma^{\text{sr}} - \bar{z})^{-1} \| \leq C(e, \Lambda) \frac{1 \vee |\operatorname{Re} z|}{1 \wedge |\operatorname{Im} z|}.$$

Putting these remarks together we arrive at the asserted bound on $W_R^F(z)$ for the SRPF operator.

In the case of the no-pair operator

$$(4.4) \quad \begin{aligned} [\chi_R, H_{\gamma,R}^{\text{np}}] e^F &= [\chi_R, |D_{\mathbf{A}}|] e^F + \frac{1}{2} [\chi_R, S_{\mathbf{A}}] e^F H_f e^{-F} S_{\mathbf{A}} e^F + \frac{1}{2} S_{\mathbf{A}} H_f [\chi_R, S_{\mathbf{A}}] e^F \\ &\quad + \frac{1}{2} [\chi_R, S_{\mathbf{A}}] e^F V_{\gamma,R} e^{-F} S_{\mathbf{A}} e^F + \frac{1}{2} S_{\mathbf{A}} V_{\gamma,R} [\chi_R, S_{\mathbf{A}}] e^F. \end{aligned}$$

The first term on the RHS of (4.4) is dealt with exactly as in the case of the SRPF operator above. Moreover, on account of (4.3) and $\| e^{-F} S_{\mathbf{A}} e^F \| \leq C(a)$ (see (A.7)) the norms of both operators in the third line of (4.4) are bounded by some constant depending only on a and R . By Lemma A.4 we finally have

$$\| (H_f + 1)^{-1} [\chi_R, S_{\mathbf{A}}] e^F H_f \| \leq C(a, e, \Lambda) \| \nabla \chi_R e^F \|_\infty \leq C(a, e, \Lambda) \frac{\|\nabla \chi\| e^{4aR}}{R},$$

and we conclude by means of the following consequence of (3.9),

$$\| H_f S_{\mathbf{A}} (H_\gamma^{\text{np}} - \bar{z})^{-1} \| = \| H_f (H_\gamma^{\text{np}} - \bar{z})^{-1} \| \leq C(e, \Lambda) \frac{1 \vee |\operatorname{Re} z|}{1 \wedge |\operatorname{Im} z|}.$$

Here we also use that $[H_\gamma^{\text{np}}, S_{\mathbf{A}}] = 0$. ■

LEMMA 4.2. For all $z \in \mathbb{C} \setminus \mathbb{R}$, $R \geq 1$, $F \in \mathcal{W}_a$, and $a \in (0, 1)$,

$$\chi_R (H - z)^{-1} - (H_R - z)^{-1} \chi_R = (H_R - z)^{-1} e^{-F} (U_R^F(z)^* + W_R^F(z)^*).$$

Proof. For all $\varphi \in \mathcal{D}$,

$$\begin{aligned} & \{ (H - z)^{-1} \chi_R - \chi_R (H_R - z)^{-1} \} (H_R - z) \varphi \\ &= (H - z)^{-1} \chi_R (H_R - z) \varphi - \chi_R \varphi \\ &= (H - z)^{-1} (H_R - H + H - z) \chi_R \varphi - \chi_R \varphi + (H - z)^{-1} [\chi_R, H_R] \varphi \\ &= \{ (H - z)^{-1} (H_R - H) \chi_R e^F \} e^{-F} \varphi + \{ (H - z)^{-1} [\chi_R, H_R] e^F \} e^{-F} \varphi \\ &= (\overline{U}_R^F(z) + \overline{W}_R^F(z)) e^{-F} (H_R - z)^{-1} (H_R - z) \varphi. \end{aligned}$$

Now, $\overline{U}_R^F(z)$ and $\overline{W}_R^F(z)$ are bounded and $(H_R - z) \mathcal{D}$ is dense in \mathcal{H} , as H_R is essentially self-adjoint on \mathcal{D} . Hence, we infer that

$$(H - z)^{-1} \chi_R - \chi_R (H_R - z)^{-1} = (\overline{U}_R^F(z) + \overline{W}_R^F(z)) e^{-F} (H_R - z)^{-1}.$$

Taking the adjoint of this operator identity and replacing \bar{z} by z we arrive at the assertion. ■

LEMMA 4.3. For all $F \in \mathcal{W}_a$, $a \in (0, 1)$, and $\varphi \in \mathcal{D}$,

$$(4.5) \quad \operatorname{Re} \langle \varphi | e^F |D_{\mathbf{A}}| e^{-F} \varphi \rangle \geq \langle \varphi | (D_{\mathbf{A}}^2 - |\nabla F|^2)^{1/2} \varphi \rangle.$$

Proof. For every non-negative operator, $T \geq 0$, on some Hilbert space and $\psi \in \mathcal{D}(T)$, we have

$$T^{1/2} \psi = \int_0^\infty (T + \eta)^{-1} T \psi \frac{d\eta}{\pi \eta^{1/2}} = \int_0^\infty (\mathbf{1} - \eta (T + \eta)^{-1}) \psi \frac{d\eta}{\pi \eta^{1/2}}.$$

For every $\varphi \in \mathcal{D}$, this yields the formula

$$\langle \varphi | (e^F |D_{\mathbf{A}}| e^{-F} - (D_{\mathbf{A}}^2 - |\nabla F|^2)^{1/2}) \varphi \rangle = \int_0^\infty J[\varphi; \eta] \frac{\eta^{1/2} d\eta}{\pi},$$

with

$$J[\varphi; \eta] := \langle \varphi | (\mathcal{R}_F(\eta) - e^F \mathcal{R}_0(\eta) e^{-F}) \varphi \rangle, \quad \mathcal{R}_G(\eta) := (D_{\mathbf{A}}^2 - |\nabla G|^2 + \eta)^{-1}, \quad G \in \{0, F\}.$$

Now, let $\phi := e^F (D_{\mathbf{A}}^2 + \eta) e^{-F} \psi$, for some $\psi \in \mathcal{D}$. Then

$$\begin{aligned} \operatorname{Re} \langle \phi | e^F \mathcal{R}_0(\eta) e^{-F} \phi \rangle &= \operatorname{Re} \langle e^F (D_{\mathbf{A}}^2 + \eta) e^{-F} \psi | \psi \rangle \\ &= \langle (D_{\mathbf{A}}^2 - |\nabla F|^2 + \eta) \psi | \psi \rangle \geq (1 - a^2 + \eta) \|\psi\|^2 \geq 0. \end{aligned}$$

It is well-known that $D_{\mathbf{A}}^2$ is essentially selfadjoint on \mathcal{D} . Since, for every $F \in \mathcal{W}_a$, multiplication with e^{-F} maps \mathcal{D} bijectively onto itself, this implies that $(D_{\mathbf{A}}^2 + \eta) e^{-F} \mathcal{D}$ is dense in \mathcal{H} . Since $F \in \mathcal{W}_a$ is bounded we conclude that the previous

estimates hold, for all ϕ in some dense domain, whence $\text{Re} [e^F \mathcal{R}_0(\eta) e^{-F}] \geq 0$ as a quadratic form on \mathcal{H} . Next, we set $Q := (\alpha \cdot \nabla F) D_{\mathbf{A}} + D_{\mathbf{A}} (\alpha \cdot \nabla F)$ and let

$$\varphi := (D_{\mathbf{A}}^2 - |\nabla F|^2 + \eta) \psi = e^{\pm F} (D_{\mathbf{A}}^2 + \eta) e^{\mp F} \psi \mp iQ \psi,$$

for $\psi \in \mathcal{D}$. Then

$$J[\varphi; \eta] = i \langle e^{-F} \mathcal{R}_0(\eta) e^F \varphi | Q \psi \rangle = i \langle \psi | Q \psi \rangle + \langle Q \psi | e^F \mathcal{R}_0(\eta) e^{-F} Q \psi \rangle.$$

Here $D_{\mathbf{A}}^2 - |\nabla F|^2$ is essentially selfadjoint on \mathcal{D} and Q is symmetric on the same domain. Hence, $\text{Re} J[\varphi; \eta] \geq 0$, for all φ in a dense set, thus for all $\varphi \in \mathcal{H}$, and we conclude. ■

In what follows we set

$$(4.6) \quad \rho(a) := 1 - (1 - a^2)^{1/2}, \quad a \in (0, 1).$$

LEMMA 4.4. For all $\delta > 0$, $a \in (0, 1)$, and $R \geq 1$,

$$\sup \left\{ \|e^F (H_R - z)^{-1} e^{-F}\| : F \in \mathcal{W}_a, \text{Re } z \leq \Sigma - \rho(a) - \frac{g}{R} - h a^2 - \delta \right\} \leq \frac{1}{\delta},$$

where $g = \gamma$ and $h = 0$ in the case of the SRPF operator. In the case of the no-pair operator we may choose $g, h = C(a, e, \Lambda)$.

Proof. It suffices to show that, for $\text{Re } z \leq \Sigma - \rho(a) - g/R - h a^2 - \delta$ and all $\psi \in \mathcal{D}$,

$$(4.7) \quad \delta \|\psi\|^2 \leq \text{Re} \langle \psi | e^F (H_R - z) e^{-F} \psi \rangle \leq \|\psi\| \|e^F (H_R - z) e^{-F} \psi\|.$$

In fact, if $F \in \mathcal{W}_a$, then e^{-F} maps \mathcal{D} bijectively onto itself, thus $(H_R - z) e^{-F} \mathcal{D}$ is dense in \mathcal{H} , as we know that H_R is essentially self-adjoint on \mathcal{D} and $z \in \rho(H_R)$. In particular, we may insert $\psi := e^F (H_R - z)^{-1} e^{-F} \varphi$, $\varphi \in \mathcal{H}$, into (4.7), since $F \in \mathcal{W}_a$ is bounded, and this yields the assertion.

First, we prove (4.7) for the SRPF operator. Since the square root is operator monotone, $|\nabla F| \leq a$, and $|D_{\mathbf{A}}| \geq 1$, we have

$$(D_{\mathbf{A}}^2 - |\nabla F|^2)^{1/2} \geq |D_{\mathbf{A}}| + (D_{\mathbf{A}}^2 - a^2)^{1/2} - |D_{\mathbf{A}}| \geq |D_{\mathbf{A}}| - \rho(a).$$

Applying (4.5) we deduce that, as quadratic forms on \mathcal{D} ,

$$\begin{aligned} \text{Re} [e^F H_{\gamma, R}^{\text{sr}} e^{-F}] &= \text{Re} [e^F |D_{\mathbf{A}}| e^{-F}] + V_{\gamma, R} + H_f \geq |D_{\mathbf{A}}| + H_f - \rho(a) + V_{\gamma, R} \\ &\geq \Sigma^{\text{sr}} - \rho(a) - \frac{\gamma}{R}. \end{aligned}$$

In order to discuss the no-pair operator we put

$$S_{\mathbf{A}}^F := e^F S_{\mathbf{A}} e^{-F}, \quad \mathcal{K}_F := [e^F, S_{\mathbf{A}}] e^{-F}, \quad \pm F \in \mathcal{W}_a.$$

According to Lemma 3.5 of [24] (or Lemma A.3) we have $\|S_{\mathbf{A}}^F\| = O(1)$ and $\|\mathcal{K}_F\| = O(a)$, as $a \searrow 0$. We further define

$$\Delta(H_f) := e^F S_{\mathbf{A}} H_f S_{\mathbf{A}} e^{-F} - S_{\mathbf{A}} H_f S_{\mathbf{A}} = S_{\mathbf{A}} H_f \mathcal{K}_F + \mathcal{K}_F H_f S_{\mathbf{A}} + \mathcal{K}_F H_f \mathcal{K}_F.$$

Then a brief computation using (3.6) gives

$$e^F H_{\gamma,R}^{\text{np}} e^{-F} = e^F |D_{\mathbf{A}}| e^{-F} + \frac{1}{2}(V_{\gamma,R} + H_f + S_{\mathbf{A}} H_f S_{\mathbf{A}}) + \frac{1}{2} S_{\mathbf{A}}^F V_{\gamma,R} S_{\mathbf{A}}^F + \frac{1}{2} \Delta(H_f)$$

on \mathscr{D} , and similarly as above we obtain

$$\text{Re} [e^F H_{\gamma,R}^{\text{np}} e^{-F}] \geq H_0^{\text{np}} - \rho(a) - \frac{\mathcal{O}(1)}{R} + \frac{\text{Re} \Delta(H_f)}{2}$$

on \mathscr{D} . Furthermore,

$$\begin{aligned} & 2 |\langle \varphi | \text{Re} \Delta(H_f) \varphi \rangle| \\ & \leq a^2 \|H_f^{1/2} S_{\mathbf{A}} \varphi\|^2 + \frac{1}{a^2} \|H_f^{1/2} (\mathcal{K}_F + \mathcal{K}_F^*) \varphi\|^2 + \|H_f^{1/2} \mathcal{K}_F \varphi\|^2 + \|H_f^{1/2} \mathcal{K}_F^* \varphi\|^2 \\ & \leq a^2 C(a, e, \Lambda) \langle \varphi | H_0^{\text{np}} \varphi \rangle, \end{aligned}$$

for all $\varphi \in \mathscr{D}$, where we used $\mathcal{K}_F^* = \mathcal{K}_{-F}$ and

$$(4.8) \quad \|H_f^{1/2} \mathcal{K}_{\pm F} (H_f + 1)^{-1/2}\|^2 + \|H_f^{1/2} (\mathcal{K}_F + \mathcal{K}_F^*) (H_f + 1)^{-1/2}\|^2 \leq C'(a, e, \Lambda) a^2,$$

in the second step. The bound (4.8) follows from (A.12) and (A.13) below. In fact, $\mathcal{K}_F + \mathcal{K}_F^*$ is equal to the double commutator in (A.13). Therefore,

$$\begin{aligned} \text{Re} [e^F H_{\gamma,R}^{\text{np}} e^{-F}] & \geq (1 - \mathcal{O}(a^2)) H_0^{\text{np}} - \rho(a) - \frac{\mathcal{O}(1)}{R} \\ & \geq \Sigma^{\text{np}} - \rho(a) - \frac{\mathcal{O}(1)}{R} - \mathcal{O}(a^2) \Sigma^{\text{np}}, \quad a \searrow 0. \quad \blacksquare \end{aligned}$$

In the following theorem, which is our first main result, we denote the spectral family of some self-adjoint operator, T , as $\mathbb{R} \ni \lambda \mapsto \mathbf{1}_\lambda(T)$.

THEOREM 4.5 (Exponential localization). *Let $e \in \mathbb{R}$, $\Lambda > 0$, and define $\rho(a)$ by (4.6). Then the following assertions hold true:*

(i) *For all $\lambda < \Sigma^{\text{sr}}$, $a \in (0, 1)$ with $\Sigma^{\text{sr}} - \lambda > \rho(a)$, and $\gamma \in (0, \gamma_c^{\text{sr}}]$, we have $\text{Ran}(\mathbf{1}_\lambda(H_\gamma^{\text{sr}})) \subset \mathcal{D}(e^{a|\tilde{x}|})$ and*

$$\|e^{a|\tilde{x}|} \mathbf{1}_\lambda(H_\gamma^{\text{sr}})\| \leq C(a, \lambda, e, \Lambda).$$

(ii) *There is some $c(e, \Lambda) > 0$, such that, for all $\lambda < \Sigma^{\text{np}}$, $a \in (0, 1)$ satisfying $\Sigma^{\text{np}} - \rho(a) - c(e, \Lambda) a^2 > \lambda$, and $\gamma \in (0, \gamma_c^{\text{np}}]$, we have $\text{Ran}(\mathbf{1}_\lambda(H_\gamma^{\text{np}})) \subset \mathcal{D}(e^{a|\tilde{x}|})$ and*

$$\|e^{a|\tilde{x}|} \mathbf{1}_\lambda(H_\gamma^{\text{np}})\| \leq C'(a, \lambda, e, \Lambda).$$

Proof. We treat both models simultaneously again using the notation (4.2) and the quantities g and h appearing in the statement of Lemma 4.4.

We put $\Delta := \Sigma - \rho(a) - h a^2 - \lambda$ and choose $R \geq 1 \vee (3/\Delta)$ large enough such that $g/R < \Delta/3$. Then $H_R \geq \Sigma - \|V_{\gamma,R}\|_\infty \geq \Sigma - \Delta/3$; recall (4.1). Furthermore, we pick some $f \in C_0^\infty(\mathbb{R}, [0, 1])$ satisfying $f = 1$ on $[E, \lambda]$ and $f = 0$ on $\mathbb{R} \setminus (E - 1, \lambda + \Delta/3)$, so that $f(H_R) = 0$, thus

$$(4.9) \quad \chi_R \mathbf{1}_\lambda(H) = (\chi_R f(H) - f(H_R) \chi_R) \mathbf{1}_\lambda(H).$$

(This identity with χ_R replaced by 1 is observed in [1] for similar purposes.) As in [1] we extend f almost analytically to some $f \in C_0^\infty(\mathbb{C})$ with

$$\begin{aligned} \text{supp}(f) &\subset [E - 1, \lambda + \Delta/3] + i[-1, 1], \\ |\partial_{\bar{z}}f(z)| &\leq C(\Delta, N) |\text{Im } z|^N, \quad z \in \mathbb{C}, \quad N \in \mathbb{N}, \end{aligned}$$

and apply the Helffer–Sjöstrand formula,

$$f(T) = \int_{\mathbb{C}} (T - z)^{-1} d\mu(z), \quad d\mu(z) := \frac{1}{2\pi i} \partial_{\bar{z}}f(z) dz \wedge d\bar{z},$$

which is valid, for any self-adjoint operator T in some Hilbert space; see, e.g., [5]. Combining it with (4.9) and Lemma 4.2 we obtain, for every $F \in \mathscr{W}_a$,

$$\begin{aligned} \chi_R e^F \mathbf{1}_\lambda(H) &= \int_{\mathbb{C}} e^F (\chi_R (H - z)^{-1} - (H_R - z)^{-1} \chi_R) \mathbf{1}_\lambda(H) d\mu(z) \\ &= \int_{\mathbb{C}} e^F (H_R - z)^{-1} e^{-F} (U_R^F(z)^* + W_R^F(z)^*) \mathbf{1}_\lambda(H) d\mu(z). \end{aligned}$$

Applying Lemma 4.1 and Lemma 4.4 (with $\delta = \Delta/3$) we arrive at

$$\sup_{F \in \mathscr{W}_a} \|\chi_R e^F \mathbf{1}_\lambda(H)\| \leq \frac{C(a, e, \Lambda, R)}{\Delta} \int_{\mathbb{C}} \frac{|\partial_{\bar{z}}f(z)|}{|\text{Im } z|} |dz \wedge d\bar{z}| \leq C(a, e, \Lambda, \Delta).$$

To conclude we pick a sequence $F_n \in \mathscr{W}_a$, $n \in \mathbb{N}$, converging monotonically to $a|\mathbf{x}| - a$ on $\{|\mathbf{x}| \geq 2\}$. Then, by monotone convergence, $\int_{\mathbb{R}^3} e^{2a|\mathbf{x}|} \|\psi(\mathbf{x})\|_{\mathscr{F}_b^4}^2 d^3\mathbf{x} =$

$$\lim_{n \rightarrow \infty} \int_{\mathbb{R}^3} e^{2F_n(\mathbf{x})} \|\psi(\mathbf{x})\|_{\mathscr{F}_b^4}^2 d^3\mathbf{x} \leq C'(a, e, \Lambda, \Delta), \quad \psi \in \text{Ran}(\mathbf{1}_\lambda(H)) \subset \int_{\mathbb{R}^3}^\oplus \mathscr{F}_b^4 d^3\mathbf{x}. \quad \blacksquare$$

In the non-relativistic setting an analog of Theorem 4.5 has been obtained in [1], [9]. Let Σ^{nr} denote the ionization threshold of the NRPF Hamiltonian. Then the decay rate found in [9] for the localization of states of energy $\leq \lambda < \Sigma^{\text{nr}}$ is $a^2 < \Sigma^{\text{nr}} - \lambda$. Together with a bound on the increase of binding energy in the NRPF model (compared to the case $e = 0$) it actually shows that the localization of the lowest energy states is improved in presence of a quantized radiation field. In case of the SRPF model the bound on the rate a in Theorem 4.5(i) is good enough to demonstrate the same effect. To explain these issues more precisely we first consider the case without radiation field.

If we set the parameter e equal to zero and restrict the operators H_γ^{sr} and H_γ^+ to the vacuum sector, then we get back the electronic operators defined in (3.1) and (3.4), respectively. In particular, we may observe the following (to the largest part well-known) result:

COROLLARY 4.6. *Let γ_c be γ_c^{sr} or γ_c^{np} and H_γ^{el} be $H_\gamma^{\text{el, sr}}$ or $H_\gamma^{\text{el, np}}$. Then, for all $\gamma \in (0, \gamma_c]$, $\lambda \in [0, 1)$, and $a > 0$ with $a^2 < 1 - \lambda^2$, we have $\text{Ran}(\mathbf{1}_\lambda(H_\gamma^{\text{el}})) \subset \mathcal{D}(e^{a|\tilde{\mathbf{x}}|})$ and*

$$\|e^{a|\tilde{\mathbf{x}}|} \mathbf{1}_\lambda(H_\gamma^{\text{el}})\| \leq C(a, \lambda).$$

Proof. First, we recall that $\Sigma^{\text{sr}}|_{e=0} = \Sigma^{\text{np}}|_{e=0} = 1$. Hence, if $H_\gamma^{\text{el}} = H_\gamma^{\text{el, sr}}$, then the assertion of the corollary is contained in the statement of Theorem 4.5(i). If $H_\gamma^{\text{el}} = H_\gamma^{\text{el, np}}$, then the assertion of the corollary can be verified by inspection of the proofs in the present section. In fact, if we ignore all Fock space operators, then we may choose $h = 0$ in Lemma 4.4 also when we consider the electronic no-pair model. As a consequence, the constant $c(e, \Lambda)$ appearing in the statement of Theorem 4.5(ii) can be replaced by zero. ■

For the no-pair model the statement of Corollary 4.6 is a special case of a result in [23], where also non-vanishing classical magnetic fields are considered. For the square root operator the assertion of Corollary 4.6 is well-known, at least for all $\gamma \in (0, 1/2]$ [27]; see also [4], [13] for exponential decay estimates for square-root operators. As it seems to us the whole range of allowed γ is not covered by the published literature so far. The bound on the decay rate $a^2 < 1 - \lambda^2$ is familiar from the analysis of the Dirac operator.

REMARK 4.7 (On improved localization due to the radiation field). Let $e_\gamma := \inf \sigma[H_\gamma^{\text{el, sr}}]$, $\gamma \in (0, \gamma_c^{\text{sr}}]$, denote the value of the lowest eigenvalue of the electronic square root operator. It is known that $0 < e_\gamma < 1$, for all $\gamma \in (0, \gamma_c^{\text{sr}}]$. In fact, strict positivity of $e_{\gamma_c^{\text{sr}}}$ is shown numerically in [12] and it is proven analytically in [29]. Then the value $a_\gamma := (1 - e_\gamma^2)^{1/2} \in (0, 1)$ is the border line for all decay rates a allowed for in Corollary 4.6. Corresponding pointwise lower bounds for ground state eigenfunctions of square root operators (whose potentials belong to a suitable Kato class) [4] suggest a_γ to be optimal indeed. Now, assume that, for $e \neq 0$ and $\Lambda > 0$, the *binding energy is increased* in the SRPF model, i.e. assume the *strict inequality*

$$(4.10) \quad \Sigma^{\text{sr}} - E_\gamma^{\text{sr}} > 1 - e_\gamma.$$

Since $1 - e_\gamma = 1 - (1 - a_\gamma^2)^{1/2} = \rho(a_\gamma)$ we conclude by means of Theorem 4.5(i) that in this case

$$\forall \gamma \in (0, \gamma_c^{\text{sr}}] \quad \exists \varepsilon > 0 : \quad \|e^{(a_\gamma + \varepsilon)|\hat{x}|} \mathbf{1}_{\{E_\gamma\}}(H_\gamma^{\text{sr}})\| \leq C(e, \Lambda, \varepsilon).$$

Thus, we observe an enhancement of localization in the ground state due to the quantized radiation field. The condition (4.10) is verified by the present authors in a separate paper [16].

5. GROUND STATES AT CRITICAL COUPLING

Starting from the assertions of Propositions 3.1(ii) and 3.2(ii), namely that H_γ^{sr} and H_γ^{np} have eigenvalues at the bottom of their spectra, as long as γ is subcritical, we prove in this section that both operators still possess ground state eigenvectors, when γ attains the critical values γ_c^{sr} and γ_c^{np} , respectively.

We shall make use of the following abstract lemma which is a variant of a result we learned from [1]; see Lemma 5.1 of [17] for a proof.

LEMMA 5.1. *Let T, T_1, T_2, \dots be self-adjoint operators acting in some separable Hilbert space, \mathcal{X} , such that $\{T_j\}_{j \in \mathbb{N}}$ converges to T in the strong resolvent sense. Assume that E_j is an eigenvalue of T_j with corresponding eigenvector $\phi_j \in \mathcal{D}(T_j)$. If $\{\phi_j\}_{j \in \mathbb{N}}$ converges weakly to some $0 \neq \phi \in \mathcal{X}$, then $E := \lim_{j \rightarrow \infty} E_j$ exists and is an eigenvalue of T . If $E_j = \inf \sigma[T_j]$, then T is semi-bounded below and $E = \inf \sigma[T]$.*

As we wish to consider the limit as γ approaches its critical values we employ the following new convention from now on:

$$(5.1) \quad \left\{ \begin{array}{l} \text{The symbols } H_\gamma, \Sigma, E_\gamma, \gamma_c \text{ denote either} \\ H_\gamma^{\text{sr}}, \Sigma^{\text{sr}}, E_\gamma^{\text{sr}}, \gamma_c^{\text{sr}} \text{ or } H_\gamma^{\text{np}}, \Sigma^{\text{np}}, E_\gamma^{\text{np}}, \gamma_c^{\text{np}}. \end{array} \right.$$

LEMMA 5.2. *H_γ converges to H_{γ_c} in the strong resolvent sense, as $\gamma \nearrow \gamma_c$. In particular,*

$$(5.2) \quad \limsup_{\gamma < \gamma_c} E_\gamma \leq E_{\gamma_c}.$$

Proof. For every $\gamma \in (0, \gamma_c)$, we know that $\mathcal{Q}(H_\gamma) = \mathcal{Q}(|D_0|) \cap \mathcal{Q}(H_f) \subset \mathcal{Q}(H_{\gamma_c})$ [18]. Since \mathcal{D} is a form core for H_{γ_c} we thus have $\overline{\bigcap_{\gamma < \gamma_c} \mathcal{Q}(H_\gamma)} = \mathcal{Q}(H_{\gamma_c})$, where the closure is taken with respect to the form norm of H_{γ_c} . Since the expectation values $\langle \varphi | H_\gamma \varphi \rangle \searrow \langle \varphi | H_{\gamma_c} \varphi \rangle$ converge monotonically, as $\gamma \nearrow \gamma_c$, for every $\varphi \in \bigcap_{\gamma < \gamma_c} \mathcal{Q}(H_\gamma) = \mathcal{Q}(|D_0|) \cap \mathcal{Q}(H_f)$, it follows from Satz 9.23a of [34] that H_γ converges to H_{γ_c} in the strong resolvent sense. ■

In order to verify the assumption $\phi \neq 0$ of Lemma 5.1 we shall adapt a compactness argument from [10]. To this end we need the infra-red bounds of the next proposition which give some information on the localization and the weak derivatives of ground state eigenvectors with respect to the photon variables. In non-relativistic QED soft photon bounds (without infra-red regularization) have been obtained first in [2] and photon derivative bounds have been introduced in [10]. To state these bounds for our models we recall 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, for $\psi = (\psi^{(n)})_{n=0}^\infty \in \mathcal{F}_b[\mathcal{X}]$, and $a(k) (\psi^{(0)}, 0, 0, \dots) = 0$.

PROPOSITION 5.3 (Infra-red bounds). *Let $e \in \mathbb{R}$, $\Lambda > 0$, and $\gamma_1 \in (0, \gamma_c)$. Then there is some $C(e, \Lambda, \gamma_1) \in (0, \infty)$, such that, for all $\gamma \in [\gamma_1, \gamma_c)$ and every normalized ground state eigenvector, ϕ_γ , of H_γ , we have the soft photon bound,*

$$(5.3) \quad \|a(k) \phi_\gamma\|^2 \leq \mathbf{1}_{\{|\mathbf{k}| \leq \Lambda\}} \frac{C(e, \Lambda, \gamma_1)}{|\mathbf{k}|},$$

for almost every $k = (\mathbf{k}, \lambda) \in \mathbb{R}^3 \times \mathbb{Z}_2$, and the photon derivative bound,

$$(5.4) \quad \|a(\mathbf{k}, \lambda) \phi_\gamma - a(\mathbf{p}, \lambda) \phi_\gamma\| \leq C(e, \Lambda, \gamma_1) |\mathbf{k} - \mathbf{p}| \left(\frac{1}{|\mathbf{k}|^{1/2} |\mathbf{k}_\perp|} + \frac{1}{|\mathbf{p}|^{1/2} |\mathbf{p}_\perp|} \right),$$

for almost every $\mathbf{k}, \mathbf{p} \in \mathbb{R}^3$ with $0 < |\mathbf{k}| < \Lambda$, $0 < |\mathbf{p}| < \Lambda$, and $\lambda \in \mathbb{Z}_2$. (Here we use the notation (2.3).) In particular, we have the following, where $\phi_\gamma = (\phi_\gamma^{(n)})_{n=0}^\infty \in \bigoplus_{n=0}^\infty L^2(\mathbb{R}^3, \mathbb{C}^4) \otimes \mathcal{F}_b^{(n)}[\mathcal{H}]$:

$$(5.5) \quad \sup_{\gamma \in [\gamma_1, \gamma_c)} \sum_{n=1}^\infty n \|\phi_\gamma^{(n)}\|^2 < \infty.$$

Proof. First, we prove the soft photon bound (5.3) for the SRPF operator. To this end we put

$$R_A(iy) := (D_A - iy)^{-1}, \quad y \in \mathbb{R}, \quad \mathcal{R}_k := (H_\gamma^{\text{sr}} - E_\gamma^{\text{sr}} + |\mathbf{k}|)^{-1}, \quad \mathbf{k} \neq 0,$$

and (recall (2.5))

$$\tilde{\mathbf{G}}_x(k) := \mathbf{G}_x(k) - \mathbf{G}_0(k) = \mathbf{G}_0(k) (e^{-i\mathbf{k} \cdot \mathbf{x}} - 1).$$

For $\gamma \in (0, \gamma_c^{\text{sr}})$, we derived the following representation in [17],

$$a(k) \phi_\gamma := i(|\mathbf{k}| \mathcal{R}_k - 1) \mathbf{G}_0(k) \cdot \hat{\mathbf{x}} \phi_\gamma - \mathcal{R}_k \alpha \cdot \tilde{\mathbf{G}}_{\hat{\mathbf{x}}}(k) S_A \phi_\gamma + I_\gamma(k),$$

for almost every $k = (\mathbf{k}, \lambda) \in \mathbb{R}^3 \times \mathbb{Z}_2$, where

$$I_\gamma(k) := \int_{\mathbb{R}} \mathcal{R}_k D_A R_A(iy) \alpha \cdot \tilde{\mathbf{G}}_{\hat{\mathbf{x}}}(k) R_A(iy) \phi_\gamma \frac{dy}{\pi}.$$

Here the Bochner integral $I_\gamma(k)$ is actually absolutely convergent. In fact, pick some $F \in C^\infty(\mathbb{R}_x^3, [0, \infty))$ such that $F(\mathbf{x}) = a|\mathbf{x}|$, for large $|\mathbf{x}|$, and $|\nabla F| \leq a$. In view of Theorem 4.5 we may choose $a \in (0, 1/2]$ sufficiently small (depending on γ_1) such that $\sup_{\gamma \in [\gamma_1, \gamma_c^{\text{sr}})} \|e^F \phi_\gamma\| < \infty$. By virtue of (3.8) and Theorem 4.5 we then

obtain, for all $\gamma \in [\gamma_1, \gamma_c^{\text{sr}})$,

$$\begin{aligned} \|I_\gamma(k)\| &\leq \int_{\mathbb{R}} \left\{ \| |D_A|^{1/4} \mathcal{R}_k \| \| |D_A|^{3/4} R_A(iy) \| \right. \\ &\quad \left. \cdot |\mathbf{G}_0(k)| \sup_x |(e^{-i\mathbf{k} \cdot \mathbf{x}} - 1) e^{-F(\mathbf{x})}| \|e^F R_A(iy) e^{-F}\| \|e^F \phi_\gamma\| \right\} \frac{dy}{\pi}, \end{aligned}$$

Here $\| |D_A|^{1/4} \mathcal{R}_k \| \leq C(e, \Lambda) / (1 \wedge |\mathbf{k}|)$ by (3.8), $\| |D_A|^{3/4} R_A(iy) \| \leq C \langle y \rangle^{-1/4}$, and the composition $e^F R_A(iy) e^{-F}$ is well-defined with $\|e^F R_A(iy) e^{-F}\| \leq C \langle y \rangle^{-1}$ by Lemma A.1 below. Using also $|\mathbf{G}_0(k)| \leq (|e|/2\pi) |\mathbf{k}|^{-1/2} \mathbf{1}_{\{|\mathbf{k}| \leq \Lambda\}}$ as well as $|e^{-i\mathbf{k} \cdot \mathbf{x}} - 1| \leq |\mathbf{k}| |\mathbf{x}|$, we arrive at

$$\|I_\gamma(k)\| \leq \mathbf{1}_{\{|\mathbf{k}| \leq \Lambda\}} \frac{C'(e, \Lambda, \gamma_1) |\mathbf{k}|^{1/2}}{1 \wedge |\mathbf{k}|} \cdot \sup_{\gamma' \in [\gamma_1, \gamma_c^{\text{sr}})} \|e^F \phi_{\gamma'}\| \leq \mathbf{1}_{\{|\mathbf{k}| \leq \Lambda\}} \frac{C''(e, \Lambda, \gamma_1)}{|\mathbf{k}|^{1/2}},$$

for almost every $k = (\mathbf{k}, \lambda) \in \mathbb{R}^3 \times \mathbb{Z}_2$ and $\gamma \in [\gamma_1, \gamma_c^{\text{sr}})$. Now, it is also clear how to estimate the remaining terms in the formula for $a(k) \phi_\gamma$ and to get (5.3). (Notice that $\|e^F S_A \phi_\gamma\| \leq \|e^F S_A e^{-F}\| \|e^F \phi_\gamma\|$, where $\|e^F S_A e^{-F}\| \leq 1 + C a$ by (A.7) and a simple approximation argument.)

In a similar fashion we next derive the photon derivative bound (5.4) for the SRPF operator. In fact, $\|(\mathcal{R}_k - \mathcal{R}_p) \psi\| \leq |\mathbf{p}|^{-1} |\mathbf{k} - \mathbf{p}| \|\mathcal{R}_k \psi\|$, $\psi \in \mathcal{H}$, by the first resolvent identity, thus

$$\begin{aligned} & \|I_\gamma(\mathbf{k}, \lambda) - I_\gamma(\mathbf{p}, \lambda)\| \\ & \leq \int_{\mathbb{R}} \left\{ \| |D_A|^{1/4} \mathcal{R}_k \| \| |D_A|^{3/4} R_A(iy) \| \right. \\ & \quad \cdot \sup_x \{ |\tilde{\mathbf{G}}_x(\mathbf{k}, \lambda) - \tilde{\mathbf{G}}_x(\mathbf{p}, \lambda)| e^{-F(x)} \} \|e^F R_A(iy) e^{-F}\| \|e^F \phi_\gamma\| \} \frac{dy}{\pi} \\ & \quad + \frac{|\mathbf{k} - \mathbf{p}|}{|\mathbf{p}|} \int_{\mathbb{R}} \left\{ \| |D_A|^{1/4} \mathcal{R}_k \| \| |D_A|^{3/4} R_A(iy) \| \right. \\ & \quad \cdot \sup_x \{ |\tilde{\mathbf{G}}_x(\mathbf{p}, \lambda)| e^{-F(x)} \} \|e^F R_A(iy) e^{-F}\| \|e^F \phi_\gamma\| \} \frac{dy}{\pi}. \end{aligned}$$

Here $|\tilde{\mathbf{G}}_x(\mathbf{p}, \lambda)| \leq (|e|/2\pi) |\mathbf{p}|^{1/2} |\mathbf{x}| \mathbf{1}_{\{|\mathbf{p}| \leq \Lambda\}}$ and some elementary estimates [10] (see also Section 6.3 of [17]) using the special choice (2.4) of the polarization vectors reveal that

$$(5.6) \quad \frac{|\tilde{\mathbf{G}}_x(\mathbf{k}, \lambda) - \tilde{\mathbf{G}}_x(\mathbf{p}, \lambda)|}{|\mathbf{k}|} \leq C (1 + |\mathbf{x}|) |\mathbf{k} - \mathbf{p}| \left(\frac{1}{|\mathbf{k}|^{1/2} |\mathbf{k}_\perp|} + \frac{1}{|\mathbf{p}|^{1/2} |\mathbf{p}_\perp|} \right),$$

provided that $0 < |\mathbf{k}|, |\mathbf{p}| < \Lambda$. By Young's inequality, also $|\mathbf{k} - \mathbf{p}| |\mathbf{k}|^{-1} |\mathbf{p}|^{-1/2}$ is bounded by the RHS of (5.6). Putting these remarks together we conclude that $\|I_\gamma(\mathbf{k}, \lambda) - I_\gamma(\mathbf{p}, \lambda)\|$ is bounded from above by the RHS of (5.4), for $0 < |\mathbf{k}|, |\mathbf{p}| < \Lambda$. Again we leave the treatment of the first two terms in the formula for $a(k) \phi_\gamma$ to the reader; we just note that $|\mathbf{k}|^{-1} |\mathbf{k}| \mathbf{G}_0(\mathbf{k}, \lambda) - |\mathbf{p}| \mathbf{G}_0(\mathbf{k}, \lambda)|$ can be bounded by the RHS of (5.6), too; see [10] or Section 6.3 of [17].

Finally, in the case of the no-pair operator we already observed in Remark 7.2 of [18] that the bound proven in Theorem 4.5(ii) provides a proof of the infra-red bounds (5.3) and (5.4) with a constant independent of $\gamma \in [\gamma_1, \gamma_c^{\text{np}})$. In fact, in [18] we derived a formula for $a(k) \phi_\gamma$, when ϕ_γ is a ground state eigenvector of H_γ^{np} , $\gamma \in (0, \gamma_c)$, which comprises of more terms than in the SRPF case but is otherwise completely analogous. Hence, by essentially the same estimates as above we may derive the infra-red bounds also for the no-pair model. ■

Finally, we arrive at the principal result of this article:

THEOREM 5.4 (Ground states at critical coupling). *For $e \in \mathbb{R}$ and $\Lambda > 0$, the minima of the spectra of both $H_{\gamma_c^{\text{sr}}}^{\text{sr}}$ and $H_{\gamma_c^+}^{\text{np}}$ are eigenvalues.*

Proof. Again we treat both models simultaneously using the notation (5.1). (Recall that in view of (3.5) it suffices to show the existence of ground states for $H_{\gamma_c}^{\text{np}}$ instead of $H_{\gamma_c}^+$ in the no-pair model.)

Let ϕ_γ denote a normalized ground state eigenvector of H_γ , for every $\gamma \in (0, \gamma_c)$. Then the family $\{\phi_\gamma\}_{\gamma \in (0, \gamma_c)}$ contains some weakly convergent sequence, $\{\phi_{\gamma_j}\}_{j \in \mathbb{N}}$, $\gamma_j \nearrow \gamma_c$. We denote the weak limit of the latter by ϕ_{γ_c} . On account of Lemmata 5.1 and 5.2 it suffices to show that $\phi_{\gamma_c} \neq 0$.

With the exponential localization and infra-red bounds at hand the following compactness argument is the same as in [10] (where an artificial photon mass is removed instead), except that we first take the partial Fourier transform with respect to \mathbf{x} before we apply the Rellich–Kondrashov theorem. (If one does not exchange the roles of the electronic position and momentum coordinates then the compactness argument requires imbedding theorems for more exotic function spaces since one has to deal with fractional derivatives with respect to \mathbf{x} [17], [18]. The variant of the argument below can also be used to simplify the proofs in [17], [18].)

Let $\varepsilon > 0$. On account of (5.5) we find some $n_0 \in \mathbb{N}$ such that

$$(5.7) \quad \forall \gamma \in [\gamma_1, \gamma_c) : \sum_{n=n_0+1}^{\infty} \|\phi_\gamma^{(n)}\|^2 < \frac{\varepsilon}{2}.$$

For $n \in \mathbb{N}$, $\gamma \in (0, \gamma_c]$, and $\underline{\theta} = (\zeta, \lambda_1, \dots, \lambda_n) \in \{1, 2, 3, 4\} \times \mathbb{Z}_2^n$, we set

$$\phi_{\gamma, \underline{\theta}}^{(n)}(\mathbf{x}, \mathbf{k}_1, \dots, \mathbf{k}_n) := \phi_\gamma^{(n)}(\mathbf{x}, \zeta, \mathbf{k}_1, \lambda_1, \dots, \mathbf{k}_n, \lambda_n)$$

and denote the partial Fourier transform of $\phi_{\gamma, \underline{\theta}}^{(n)}$ with respect to \mathbf{x} as $\widehat{\phi}_{\gamma, \underline{\theta}}^{(n)}$. Then the soft photon bound (5.3) shows that $\widehat{\phi}_{\gamma, \underline{\theta}}^{(n)}(\boldsymbol{\zeta}, \mathbf{k}_1, \dots, \mathbf{k}_n) = 0$, for almost every $(\boldsymbol{\zeta}, \mathbf{k}_1, \dots, \mathbf{k}_n) \in \mathbb{R}^{3(n+1)}$, such that $|\mathbf{k}_j| > \Lambda$, for some $j \in \{1, \dots, n\}$. Moreover, pick some $s \in (0, 1)$. By virtue of (3.8) we then have, for all $\gamma \in (0, \gamma_c)$, $n \in \mathbb{N}$, and every choice of $\underline{\theta}$,

$$\begin{aligned} R^s \int_{|\boldsymbol{\zeta}| \geq R} \|\widehat{\phi}_{\gamma, \underline{\theta}}^{(n)}(\boldsymbol{\zeta}, \cdot)\|_{L^2(\mathbb{R}^{3n})}^2 d^3 \boldsymbol{\zeta} &\leq \langle \phi_{\gamma, \underline{\theta}}^{(n)} | (-\Delta)^{s/2} \phi_{\gamma, \underline{\theta}}^{(n)} \rangle \\ &\leq \langle \phi_\gamma | H_\gamma \phi_\gamma \rangle + C(e, \Lambda, s) = E_\gamma + C(e, \Lambda, s) \leq |E_{\gamma_c}| + \Sigma + C(e, \Lambda, s). \end{aligned}$$

Consequently, we find some $R \geq 1$ such that

$$(5.8) \quad \sum_{n=1}^{n_0} \|\mathbf{1}_{\{|\boldsymbol{\zeta}| \geq R\}} \widehat{\phi}_\gamma^{(n)}\|^2 < \frac{\varepsilon}{2}.$$

As in [10] an application of Hölder’s inequality with respect to $d^3\boldsymbol{\zeta} d^{3(n-1)}\mathbf{K}$ and the photon derivative bound (5.4) yield, for $p \in [1, 2)$ and $\gamma \in [\gamma_1, \gamma_c)$,

$$\begin{aligned} & \int_{\substack{|\mathbf{k}| < \Lambda, \\ |\mathbf{k} + \mathbf{h}| < \Lambda}} \int \int |\widehat{\phi}_{\gamma, \underline{\theta}}^{(n)}(\boldsymbol{\zeta}, \mathbf{k} + \mathbf{h}, \mathbf{K}) - \widehat{\phi}_{\gamma, \underline{\theta}}^{(n)}(\boldsymbol{\zeta}, \mathbf{k}, \mathbf{K})|^p d^3\boldsymbol{\zeta} d^{3(n-1)}\mathbf{K} d^3\mathbf{k} \\ & \leq C \sum_{\lambda \in \mathbb{Z}_2} \int_{\substack{|\mathbf{k}| < \Lambda, \\ |\mathbf{k} + \mathbf{h}| < \Lambda}} \|a(\mathbf{k} + \mathbf{h}, \lambda) \phi_\gamma - a(\mathbf{k}, \lambda) \phi_\gamma\|^p d^3\mathbf{k} \\ & \leq C' |\mathbf{h}|^p \int_{|(u,v)| < \Lambda} \left\{ \int_0^{|(u,v)|} \frac{dr}{|(u,v)|^{p/2}} + \int_{|(u,v)|}^\Lambda \frac{dr}{r^{p/2}} \right\} \frac{du dv}{|(u,v)|^p} = C'' |\mathbf{h}|^p, \end{aligned}$$

where the constants $C, C', C'' \in (0, \infty)$ depend on p, n, e, Λ , but not on $\gamma \in [\gamma_1, \gamma_c)$. Since $\phi_\gamma^{(n)}$ is permutation symmetric with respect to the variables k_1, \dots, k_n the previous estimate implies ([28], Section 4.8) that the weak first order partial derivatives of $\widehat{\phi}_{\gamma, \underline{\theta}}^{(n)}$ with respect to its last $3n$ variables exist on $Q_n := B_R \times B_\Lambda^n$, where B_ρ denotes the open ball in \mathbb{R}^3 of radius ρ centered at the origin, and that

$$\sup_{\gamma \in [\gamma_1, \gamma_c)} \|\nabla_{\mathbf{k}_i} \widehat{\phi}_{\gamma, \underline{\theta}}^{(n)}\|_{L^p(Q_n)} < \infty, \quad p \in [1, 2), \quad i = 1, \dots, n, \quad n = 1, \dots, n_0.$$

Finally, since $\sup_{\gamma \in [\gamma_1, \gamma_c)} \|e^{a|\widehat{\mathbf{x}}|} \phi_{\gamma, \underline{\theta}}^{(n)}\| < \infty$, for some $a > 0$, we know that $\widehat{\phi}_{\gamma, \underline{\theta}}^{(n)}$ has weak first order derivatives with respect to $\boldsymbol{\zeta}$ and, for all $\gamma \in [\gamma_1, \gamma_c)$, we have

$$\begin{aligned} \|\nabla_{\boldsymbol{\zeta}} \widehat{\phi}_{\gamma, \underline{\theta}}^{(n)}\|_{L^p(Q_n)} & \leq C(p, n, R, \Lambda) \|\nabla_{\boldsymbol{\zeta}} \widehat{\phi}_{\gamma, \underline{\theta}}^{(n)}\|_{L^2(\mathbb{R}^{3(n+1)})} \\ & = C'(p, n, R, \Lambda) \|\widehat{\mathbf{x}} \phi_{\gamma, \underline{\theta}}^{(n)}\|_{L^2(\mathbb{R}^{3(n+1)})} \leq C''(p, n, R, \Lambda). \end{aligned}$$

As observed in [10] bounds with respect to the L^p -norms, $p < 2$, are actually sufficient in this situation. In fact, if we choose $p \in [1, 2)$ so large that $2 < (3(n_0 + 1)p)/(3(n_0 + 1) - p)$, then, for every $n = 1, \dots, n_0$ and every choice of $\underline{\theta}$, we may apply the Rellich–Kondrashov theorem to show that every subsequence of $\{\widehat{\phi}_{\gamma_j, \underline{\theta}}^{(n)}\}_{j \in \mathbb{N}}$ contains another subsequence which is strongly convergent in $L^2(Q_n)$. (Obviously, Q_n satisfies the required cone condition.) By finitely many repeated selections of subsequences we may hence assume without loss of generality that $\{\widehat{\phi}_{\gamma_j, \underline{\theta}}^{(n)}\}_{j \in \mathbb{N}}$ converges strongly in $L^2(Q_n)$ to $\widehat{\phi}_{\gamma_c, \underline{\theta}}^{(n)}$, for all $n = 0, \dots, n_0$ and $\underline{\theta}$. Taking (5.7) and (5.8) into account we arrive at

$$\|\phi_{\gamma_c}\|^2 = \sum_{n=0}^\infty \|\widehat{\phi}_{\gamma_c}^{(n)}\|^2 \geq \lim_{j \rightarrow \infty} \sum_{n=0}^{n_0} \sum_{\underline{\theta}} \|\widehat{\phi}_{\gamma_j, \underline{\theta}}^{(n)}\|_{L^2(Q_n)}^2 \geq \lim_{j \rightarrow \infty} \|\phi_{\gamma_j}\|^2 - \varepsilon = 1 - \varepsilon.$$

Since $\varepsilon > 0$ is arbitrary we conclude that $\|\phi_{\gamma_c}\| = 1$. ■

Appendix A. ESTIMATES ON COMMUTATORS

In this appendix we derive some bounds on the operator norms of certain commutators involving the sign function of the Dirac operator which have been used repeatedly in the main text. Except for those of Lemma A.2 all results and estimations presented here are variants of earlier ones in [24]. Nevertheless, we shall give a self-contained exposition for the convenience of the reader.

The following basic lemma, stating that the resolvent of the Dirac operator,

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

stays bounded after conjugation with suitable exponential weights, is more or less folkloric, at least in the case of classical vector potentials. The proof of (A.2) given, e.g., in [23] for classical vector potentials works for quantized ones without any changes.

LEMMA A.1. *Let $y \in \mathbb{R}$, $a \in [0, 1)$, and $F \in C^\infty(\mathbb{R}_x^3, \mathbb{R})$ such that $|\nabla F| \leq a$. Then $iy \in \varrho(D_{\mathbf{A}} + i\boldsymbol{\alpha} \cdot \nabla F)$ and*

$$(A.1) \quad R_{\mathbf{A}}^F(iy) := e^F R_{\mathbf{A}}(iy) e^{-F} = (D_{\mathbf{A}} + i\boldsymbol{\alpha} \cdot \nabla F - iy)^{-1} \quad \text{on } \mathcal{D}(e^{-F}),$$

$$(A.2) \quad \|R_{\mathbf{A}}^F(iy)\| \leq \sqrt{6} (1 - a^2)^{-1} \langle y \rangle^{-1}.$$

The factor $(1 - a^2)^{-1}$ in (A.2) will enter into many estimates below but most of the time we will absorb it into some constant. Henceforth, we stick to the convention that all constants $C(a, \dots), C'(a, \dots), \dots$ be increasing functions of a when the other displayed parameters are kept fixed.

All commutator estimates below are based on the following representation of $S_{\mathbf{A}} = D_{\mathbf{A}} |D_{\mathbf{A}}|^{-1}$ as a strongly convergent principal value,

$$(A.3) \quad S_{\mathbf{A}} \psi = \lim_{\tau \rightarrow \infty} \int_{-\tau}^{\tau} R_{\mathbf{A}}(iy) \psi \frac{dy}{\pi}, \quad \psi \in \mathcal{H}.$$

LEMMA A.2. *For every bounded $F \in C^\infty(\mathbb{R}_x^3, \mathbb{R})$ with $|\nabla F| \leq a < 1$, all $\chi \in C^\infty(\mathbb{R}_x^3, [0, 1])$ with bounded first order derivatives, and $\kappa \in [0, 1)$,*

$$\| |\hat{\mathbf{x}}|^{-\kappa} (H_f + 1)^{-1/2} [e^F S_{\mathbf{A}} e^{-F}, \chi] \| \leq C(a, e, \Lambda, \kappa) \|\nabla \chi\|_\infty.$$

Proof. To begin with we put $\check{H}_f := H_f + 1$ and observe that

$$(A.4) \quad \check{H}_f^{-1/2} R_{\mathbf{A}}^F(iy) = R_0(iy) (\check{H}_f^{-1/2} - T R_{\mathbf{A}}^F(iy)),$$

where $T \in \mathcal{L}(\mathcal{H})$ is the closure of $\check{H}_f^{-1/2} \boldsymbol{\alpha} \cdot (\mathbf{A} + i\nabla F)$ and satisfies $\|T\| \leq C(e, \Lambda)$. In fact, since $R_0(iy)$ and $\check{H}_f^{-1/2}$ commute we obtain, for every $\varphi \in \mathcal{D}$,

$$\begin{aligned} & \{ \check{H}_f^{-1/2} R_{\mathbf{A}}^F(iy) - R_0(iy) \check{H}_f^{-1/2} \} (D_{\mathbf{A}} + i\boldsymbol{\alpha} \cdot \nabla F - iy) \varphi \\ &= -R_0(iy) \check{H}_f^{-1/2} \boldsymbol{\alpha} \cdot (\mathbf{A} + i\nabla F) \varphi = -R_0(iy) T R_{\mathbf{A}}^F(iy) (D_{\mathbf{A}} + i\boldsymbol{\alpha} \cdot \nabla F - iy) \varphi. \end{aligned}$$

As $D_{\mathbf{A}}$ is essentially self-adjoint on \mathcal{D} we know that $(D_{\mathbf{A}} + i\boldsymbol{\alpha} \cdot \nabla F - iy)$ \mathcal{D} is dense in \mathcal{H} and we obtain (A.4). (In fact, if $\psi \in \mathcal{H}$ and $\varphi_n \in \mathcal{D}$ converge to $R_{\mathbf{A}}^F(iy) \psi \in \mathcal{D}(D_{\mathbf{A}})$ in the graph norm of $D_{\mathbf{A}} - iy$, then $(D_{\mathbf{A}} + i\boldsymbol{\alpha} \cdot \nabla F - iy) \varphi_n \rightarrow \psi$.) Applying the generalized Hardy inequality, $|\widehat{\mathbf{x}}|^{-2\kappa} \leq C(\kappa) |D_0|^{2\kappa}$, and $\| |D_0|^\kappa R_0(iy) \| \leq C'(\kappa) \langle y \rangle^{\kappa-1}$ we deduce from (A.2) and (A.4) that

$$\| |\widehat{\mathbf{x}}|^{-\kappa} \check{H}_f^{-1/2} R_{\mathbf{A}}^F(iy) \| \leq C''(e, \Lambda, \kappa) (1 - a^2)^{-1} \langle y \rangle^{\kappa-1}.$$

Together with (A.3), $[R_{\mathbf{A}}^F(iy), \chi] = R_{\mathbf{A}}^F(iy) i\boldsymbol{\alpha} \cdot \nabla \chi R_{\mathbf{A}}^F(iy)$, and (A.1)–(A.2) this permits to get

$$\begin{aligned} \|\langle |\widehat{\mathbf{x}}|^{-\kappa} \varphi | \check{H}_f^{-1/2} [e^F S_{\mathbf{A}} e^{-F}, \chi] \psi \rangle\| &\leq \int_{\mathbb{R}} \|\langle |\widehat{\mathbf{x}}|^{-\kappa} \varphi | \check{H}_f^{-1/2} R_{\mathbf{A}}^F(iy) i\boldsymbol{\alpha} \cdot \nabla \chi R_{\mathbf{A}}^F(iy) \psi \rangle\| \frac{dy}{\pi} \\ &\leq C'''(e, \Lambda, \kappa) (1 - a^2)^{-2} \int_{\mathbb{R}} \langle y \rangle^{\kappa-2} dy \cdot \|\nabla \chi\|_{\infty} \|\varphi\| \|\psi\|, \end{aligned}$$

for all $\varphi \in \mathcal{D}(|\widehat{\mathbf{x}}|^{-\kappa})$, $\psi \in \mathcal{H}$, and we conclude. ■

The bounds derived in the following lemma are slightly more general than the corresponding ones of Lemma 3.5 in [24].

LEMMA A.3. *Let $\kappa \in [0, 1)$, $\varepsilon > 0$, and $\chi \in C^\infty(\mathbb{R}_{\mathbf{x}}^3, [0, 1])$ with $|\nabla \chi|$ bounded. Moreover, let $F, G \in C^\infty(\mathbb{R}_{\mathbf{x}}^3, \mathbb{R})$ be bounded with bounded first order derivatives and such that $|\nabla(F - G)| \leq a < 1$. Then*

$$(A.5) \quad \| |D_{\mathbf{A}}|^\kappa [\chi e^G, S_{\mathbf{A}}] e^{F-G} \| \leq C(a, \kappa) \|(\nabla \chi + \chi \nabla G) e^F\|_{\infty},$$

$$(A.6) \quad \| |D_{\mathbf{A}}|^{-\varepsilon} [\chi e^G, |D_{\mathbf{A}}|] e^{F-G} \| \leq C(a, \varepsilon) \|(\nabla \chi + \chi \nabla G) e^F\|_{\infty}.$$

In particular, we have, for every bounded $G \in C^\infty(\mathbb{R}_{\mathbf{x}}^3, \mathbb{R})$ such that $|\nabla G| \leq a < 1$,

$$(A.7) \quad \|e^G S_{\mathbf{A}} e^{-G}\| \leq 1 + C(a) \|\nabla G\|_{\infty}.$$

Proof. Combining (A.3), the computation

$$(A.8) \quad [R_{\mathbf{A}}(iy), \chi e^G] e^{F-G} = R_{\mathbf{A}}(iy) i\boldsymbol{\alpha} \cdot (\nabla \chi + \chi \nabla G) e^F R_{\mathbf{A}}^{G-F}(iy),$$

and the bounds $\| |D_{\mathbf{A}}|^\kappa R_{\mathbf{A}}(iy) \| \leq C'(\kappa) \langle y \rangle^{\kappa-1}$ and $\| R_{\mathbf{A}}^{G-F}(iy) \| \leq C'(a) \langle y \rangle^{-1}$ we find, for all $\varphi \in \mathcal{D}(|D_{\mathbf{A}}|^\kappa)$ and $\psi \in \mathcal{H}$,

$$\begin{aligned} &\|\langle |D_{\mathbf{A}}|^\kappa \varphi | [\chi e^G, S_{\mathbf{A}}] e^{F-G} \psi \rangle\| \\ &\leq \int_{\mathbb{R}} \|\langle |D_{\mathbf{A}}|^\kappa \varphi | R_{\mathbf{A}}(iy) i\boldsymbol{\alpha} \cdot (\nabla \chi + \chi \nabla G) e^F R_{\mathbf{A}}^{G-F}(iy) \psi \rangle\| \frac{dy}{\pi} \\ (A.9) \quad &\leq C''(a, \kappa) \|(\nabla \chi + \chi \nabla G) e^F\|_{\infty} \int_{\mathbb{R}} \langle y \rangle^{\kappa-2} dy \|\varphi\| \|\psi\|, \end{aligned}$$

which gives (A.5). Choosing $\kappa = 0$, $\chi = 1$, and $F = 0$ we also obtain (A.7),

$$\|e^G S_{\mathbf{A}} e^{-G}\| \leq \|S_{\mathbf{A}}\| + \| [e^G, S_{\mathbf{A}}] e^{-G} \| \leq 1 + C(a) \|\nabla G\|_{\infty}.$$

To derive (A.6) we write $|D_{\mathbf{A}}| = D_{\mathbf{A}} S_{\mathbf{A}}$ and compute

$$[\chi e^G, |D_{\mathbf{A}}|] e^{F-G} = i\alpha \cdot (\nabla\chi + \chi \nabla G) e^F (e^{G-F} S_{\mathbf{A}} e^{F-G}) + D_{\mathbf{A}} [\chi e^G, S_{\mathbf{A}}] e^{F-G}$$

on \mathcal{D} . (Thanks to proof of Lemma 3.4(ii) in [24] we know that $S_{\mathbf{A}}$ maps $e^{F-G} \mathcal{D} = \mathcal{D}$ into $\mathcal{D}(D_0) \cap \mathcal{D}(H_f)$ which is left invariant under multiplication with χe^G .) Using $|D_{\mathbf{A}}|^{-\varepsilon} D_{\mathbf{A}} = S_{\mathbf{A}} |D_{\mathbf{A}}|^\kappa$ with $\kappa := 1 - \varepsilon < 1$ we thus observe that (A.6) is a consequence of (A.5) and (A.7). ■

The next lemma again presents a variant of a bound from Lemma 3.5 of [24]. In order to prove it we recall some technical tool introduced in [24]. First, we put

$$(A.10) \quad \check{H}_f := H_f + K, \quad T_\nu := [\check{H}_f^{-\nu}, \alpha \cdot \mathbf{A}] \check{H}_f^\nu \quad \text{on } \mathcal{D},$$

and recall the bound $\|T_\nu\| \leq C(e, \Lambda)/K^{1/2}$, for $\nu \geq 1/2$ and $K \geq 1$; see Lemma 3.1 of [24]. In view of (A.2) it shows that, for a sufficiently large choice of $K \geq 1$, the Neumann series $\Xi_\nu^F(y) := \sum_{\ell=0}^\infty \{-R_{\mathbf{A}}^F(iy) \bar{T}_\nu\}^\ell$ converges and satisfies, say, $\|\Xi_\nu^F(y)\| \leq 2$, for all $\nu \geq 1/2$, $y \in \mathbb{R}$, and $F \in C^\infty(\mathbb{R}_{\mathbf{x}}^3, \mathbb{R})$ with $|\nabla F| \leq a < 1$. Moreover, it is easy to verify the following useful intertwining relation ([24], Corollary 3.1):

$$(A.11) \quad \check{H}_f^{-\nu} R_{\mathbf{A}}^F(iy) = \Xi_\nu^F(y) R_{\mathbf{A}}^F(iy) \check{H}_f^{-\nu}.$$

LEMMA A.4. *Let $\nu \geq 1/2$ and χ, F , and G be as in Lemma A.3. Then*

$$(A.12) \quad \|(H_f + 1)^{-\nu} [\chi e^G, S_{\mathbf{A}}] e^{F-G} H_f^\nu\| \leq C(a, e, \Lambda)^\nu \|(\nabla\chi + \chi \nabla G) e^F\|_\infty.$$

Proof. We define \check{H}_f by (A.10), for some sufficiently large $K \geq 1$ such that the remarks preceding the statement are applicable. By means of (A.3), (A.8), and (A.11) we then obtain

$$\begin{aligned} & |\langle \varphi | \check{H}_f^{-\nu} [\chi e^G, S_{\mathbf{A}}] e^{F-G} H_f^\nu \psi \rangle| \\ & \leq \int_{\mathbb{R}} |\langle \varphi | \check{H}_f^{-\nu} R_{\mathbf{A}}(iy) i\alpha \cdot (\nabla\chi + \chi \nabla G) e^F R_{\mathbf{A}}^{G-F}(iy) H_f^\nu \psi \rangle| \frac{dy}{\pi} \\ & \leq \int_{\mathbb{R}} |\langle \varphi | \Xi_\nu^0(y) R_{\mathbf{A}}(iy) i\alpha \cdot (\nabla\chi + \chi \nabla G) e^F \Xi_\nu^{G-F}(y) R_{\mathbf{A}}^{G-F}(iy) \check{H}_f^{-\nu} H_f^\nu \psi \rangle| \frac{dy}{\pi} \\ & \leq C(a) \sup_{y \in \mathbb{R}} \{\|\Xi_\nu^0(y)\| \|\Xi_\nu^{G-F}(y)\|\} \|H_f^\nu \check{H}_f^{-\nu}\| \|(\nabla\chi + \chi \nabla G) e^F\|_\infty \int_{\mathbb{R}} \langle y \rangle^{-2} dy \\ & \leq C'(a) \|(\nabla\chi + \chi \nabla G) e^F\|_\infty, \end{aligned}$$

for all normalized $\varphi, \psi \in \mathcal{D}$. This implies (A.12) since $\|(H_f + 1)^{-\nu} \check{H}_f^\nu\| \leq K^\nu$, where our choice of K depends only on a, e , and Λ . ■

The last lemma of this appendix is just a special case of Lemma 3.6 in [24].

LEMMA A.5. For all bounded $F \in C^\infty(\mathbb{R}_x^3, \mathbb{R})$ such that $|\nabla F| \leq a < 1$ and $\nu \geq 1/2$,

$$(A.13) \quad \|(H_f + 1)^{-\nu} [e^{-F}, [S_A, e^F]] H_f^\nu\| \leq C(a, e, \Lambda)^\nu \|\nabla F\|_\infty^2.$$

Proof. A straightforward computation yields

$$[e^{-F}, [R_A(iy), e^F]] = R_A(iy) i\alpha \cdot \nabla F \{R_A^F(iy) + R_A^{-F}(iy)\} i\alpha \cdot \nabla F R_A(iy).$$

Together with (A.2), (A.3), and (A.11) this permits to get

$$\begin{aligned} & |\langle \varphi | \check{H}_f^{-\nu} [e^{-F}, [S_A, e^F]] H_f^\nu \psi \rangle| \\ & \leq 2^3 \int_{\mathbb{R}} \|R_A(iy)\| \|\nabla F\|_\infty^2 (\|R_A^F(iy)\| + \|R_A^{-F}(iy)\|) \|R_A(iy)\| \|H_f^\nu \check{H}_f^{-\nu}\| \frac{dy}{\pi} \\ & \leq C(a) \|\nabla F\|_\infty^2 \int_{\mathbb{R}} \frac{dy}{\langle y \rangle^3}, \end{aligned}$$

for all normalized $\varphi, \psi \in \mathcal{D}$. We conclude as in the previous proof. ■

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