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

## MARTIN KÖNENBERG AND OLIVER MATTE

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 which is uniform in the Coulomb coupling constant.

#### 1. Two models for a hydrogen-like atom in relativistic QED

1.1. 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. The second one is a no-pair model introduced in [12] in order to study the stability of relativistic matter interacting with the quantized radiation field. In this model the Schrödinger operators are substituted by Dirac operators and the whole Hamiltonian is restricted to a subspace

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where all electrons live in positive spectral subspaces of the free Dirac operators. In the case of a hydrogen-like atom – that is, for one electron – both models are introduced in detail in Subsection 1.3 after some notation has been fixed in Subsection 1.2. They have both been investigated in the mathematical literature before [6, 8, 11, 12, 17], but to a much lesser extend 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, respectively. In our earlier works [9, 10, 15] together with E. Stockmeyer 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, 7, 13].

Typically, in relativistic atomic models there exist critical values,  $\gamma_c$ , of the Coulomb coupling constant,  $\gamma \ge 0$ , restricting the range where physically distinguished self-adjoint realizations of the Hamiltonian can be found. (In the physical application we have  $\gamma = e^2 Z$ , where  $e^2$  is the square of the elementary charge and  $Z \ge 0$  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,  $2/(2/\pi + \pi/2)$  [4]. According to [9, 10] these critical values do not change when the interaction with the quantized photon field is taken into account. The main results of [9, 10] hold, however, only for sub-critical  $\gamma$ . Thus, 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.

Presumably it is possible to directly prove the existence of ground states along the lines of [1, 7, 9, 10], also for  $\gamma = \gamma_c$ . We think, however, that it would be quite a tedious procedure to replace all arguments in [9, 10] that exploit the sub-criticality of  $\gamma$  by alternative ones. For instance, simple characterizations of the form domains of the Hamiltonians are available, for sub-critical  $\gamma$ , which is very convenient in order to argue that certain formal computations can be justified rigorously. Therefore, it seems more convenient 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 3 similar to one used in [7] in order to remove an artificial photon mass. Among other ingredients this compactness argument requires a bound on the spatial localization of  $\phi_{\gamma}$ , which is uniform in  $\gamma < \gamma_c$ . Earlier results on the localization of low-lying spectral subspaces of the SRPF and no-pair operators provide, however, only  $\gamma$ -dependent estimates [15]. Hence, from a technical point of view the main new achievement of the present article shall be a suitable bound on the spatial exponential localization of spectral subspaces corresponding to energies below the ionization threshold which is uniform in  $\gamma \leq \gamma_c$ . This localization estimate is derived in Section 2 by suitably adapted versions of ideas in [1, 14, 15]. We remark that by now we are able to improve the localization estimates of [15] thanks to some more recent results of [10] collected in Proposition 1.3. An important requisite 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 [9, 10, 14, 15]. 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 2.4 (Exponential localization) and Theorem 3.4 (Existence of ground states at critical coupling).

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

(1.1) 
$$\mathscr{H} := L^2(\mathbb{R}^3_{\mathbf{x}}, \mathbb{C}^4) \otimes \mathscr{F}_{\mathrm{b}}[\mathscr{H}] = \int_{\mathbb{R}^3}^{\oplus} \mathbb{C}^4 \otimes \mathscr{F}_{\mathrm{b}}[\mathscr{H}] d^3 \mathbf{x} ,$$

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

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

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  $\mathscr{F}_{\mathrm{b}}^{(0)}[\mathscr{K}] := \mathbb{C}$  and, for  $n \in \mathbb{N}, \ \mathscr{F}_{\mathrm{b}}^{(n)}[\mathscr{K}] := \mathcal{S}_n L^2((\mathbb{R}^3 \times \mathbb{Z}_2)^n)$ , 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  $\{1, \ldots, n\}$ . For  $f \in \mathscr{K}$  and  $n \in \mathbb{N}_0$ , we further define  $a^{\dagger}(f)^{(n)} : \mathscr{F}_{\mathrm{b}}^{(n)}[\mathscr{K}] \to \mathscr{F}_{\mathrm{b}}^{(n+1)}[\mathscr{K}]$  by  $a^{\dagger}(f)^{(n)}\psi^{(n)} := \sqrt{n+1} \mathcal{S}_{n+1}(f \otimes \psi^{(n)})$ . Then  $a^{\dagger}(f) := \bigoplus_{n=0}^{\infty} a^{\dagger}(f)^{(n)}$  and  $a(f) := a^{\dagger}(f)^*$  are the standard bosonic creation and annihilation operators satisfying the canonical commutation relations

(1.2) 
$$[a^{\sharp}(f), a^{\sharp}(g)] = 0, \qquad [a(f), a^{\dagger}(g)] = \langle f | g \rangle \mathbb{1}, \qquad f, g \in \mathcal{K},$$

where  $a^{\sharp}$  is  $a^{\dagger}$  or a. Writing

(1.3) 
$$\mathbf{k}_{\perp} := (k^{(2)}, -k^{(1)}, 0), \quad \mathbf{k} = (k^{(1)}, k^{(2)}, k^{(3)}) \in \mathbb{R}^3,$$

we introduce two polarization vectors,

(1.4) 
$$\boldsymbol{\varepsilon}(\mathbf{k},0) = \frac{\mathbf{k}_{\perp}}{|\mathbf{k}_{\perp}|}, \quad \boldsymbol{\varepsilon}(\mathbf{k},1) = \frac{\mathbf{k}}{|\mathbf{k}|} \wedge \boldsymbol{\varepsilon}(\mathbf{k},0),$$

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

(1.5) 
$$\mathbf{G}_{\mathbf{x}}(k) = \left(G_{\mathbf{x}}^{(1)}, G_{\mathbf{x}}^{(2)}, G_{\mathbf{x}}^{(3)}\right)(k) := -e \frac{\mathbb{I}\left\{|\mathbf{k}| \le \Lambda\right\}}{2\pi |\mathbf{k}|^{1/2}} e^{-i\mathbf{k}\cdot\mathbf{x}} \boldsymbol{\varepsilon}(k),$$

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 eis the square root of Sommerfeld's fine structure constant and  $e^2 \approx 1/137$ .) For short, we write  $a^{\sharp}(\mathbf{G}_{\mathbf{x}}) := (a^{\sharp}(G_{\mathbf{x}}^{(1)}), a^{\sharp}(G_{\mathbf{x}}^{(2)}), a^{\sharp}(G_{\mathbf{x}}^{(3)}))$ . Then the quantized vector potential is the triple of operators  $\mathbf{A} = (A^{(1)}, A^{(2)}, A^{(3)})$  in  $\mathcal{H}$  given as

(1.6) 
$$\mathbf{A} := \int_{\mathbb{R}^3}^{\oplus} \mathbb{1}_{\mathbb{C}^4} \otimes \left( a^{\dagger}(\mathbf{G}_{\mathbf{x}}) + a(\mathbf{G}_{\mathbf{x}}) \right) d^3 \mathbf{x} \, .$$

The radiation field energy is the second quantization,  $H_{\rm f} := d\Gamma(\omega)$ , of the dispersion relation  $\omega : \mathbb{R}^3 \times \mathbb{Z}_2 \to \mathbb{R}$ ,  $k = (\mathbf{k}, \lambda) \mapsto \omega(k) := |\mathbf{k}|$ . 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  $\mathscr{F}_{\rm b}^{(n)}[\mathscr{K}]$  associated with the symmetric function  $(k_1, \ldots, k_n) \mapsto \omega(k_1) + \cdots + \omega(k_n)$ , if  $n \in \mathbb{N}$ .

As usual we shall consider operators in  $L^2(\mathbb{R}^3_{\mathbf{x}}, \mathbb{C}^4)$  or  $\mathscr{F}_{\mathbf{b}}[\mathscr{K}]$  also as operators acting in the tensor product  $\mathscr{H}$  by identifying  $|\hat{\mathbf{x}}|^{-1} \equiv |\hat{\mathbf{x}}|^{-1} \otimes \mathbb{1}$ ,  $H_{\mathbf{f}} \equiv \mathbb{1} \otimes H_{\mathbf{f}}$ , etc. (The 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

(1.7) 
$$\alpha_i \, \alpha_j + \alpha_j \, \alpha_i = 2 \, \delta_{ij} \, \mathbb{1}, \qquad i, j \in \{0, 1, 2, 3\}.$$

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

(1.8) 
$$D_{\mathbf{A}} := \boldsymbol{\alpha} \cdot (-i\nabla_{\mathbf{x}} + \mathbf{A}) + \alpha_0 := \sum_{j=1}^3 \alpha_j (-i\partial_{x_j} + A^{(j)}) + \alpha_0.$$

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

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

where  $\mathscr{C} \subset \mathscr{F}_{\mathbf{b}}[\mathscr{K}]$  denotes the subspace of all  $(\psi^{(n)})_{n=0}^{\infty} \in \mathscr{F}_{\mathbf{b}}[\mathscr{K}]$  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  $\mathscr{D}$ ; see, e.g., [12]. We use the symbol  $D_{\mathbf{A}}$  again to denote its closure starting from  $\mathscr{D}$ . 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  $\langle y \rangle := (1+y^2)^{1/2}, y \in \mathbb{R}$ .  $C(a,b,\ldots), C'(a,b,\ldots),\ldots$  denote positive constants which depend only on the quantities  $a, b, \ldots$  displayed in their arguments and whose values might change from one estimate to another.

1.3. The semi-relativistic Pauli-Fierz and no-pair models. In what follows we shall denote the maximal operator of multiplication with the Coulomb potential,  $-\gamma/|\mathbf{x}|$ ,  $\gamma \ge 0$ , in  $\mathscr{H}$  by  $V_{\gamma}$ . Then the semi-relativistic Pauli-Fierz (SRPF) operator is defined, a priori on the dense domain  $\mathscr{D}$ , as

$$H_{\gamma}^{\mathrm{sr}} := |D_{\mathbf{A}}| + V_{\gamma} + H_{\mathrm{f}}$$

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

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

where  $\boldsymbol{\sigma}$  is a formal vector containing the three 2×2 Pauli spin matrices. According to [10] the quadratic form associated with  $H_{\gamma}^{\rm sr}$  is semi-bounded below, if and only if  $\gamma$  is less than or equal to the critical constant in Kato's inequality,

$$\gamma_{
m c}^{
m sr}:=2/\pi$$
 .

Thus, the range of stability of  $H_{\gamma}^{\rm sr}$  is the same as the one of the purely electronic square root operator,

$$H_{\gamma}^{\mathrm{el,sr}} := \sqrt{1 - \Delta_{\mathbf{x}}} + V_{\gamma} \,.$$

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

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 [6] and the fiber decomposition of  $H_{\gamma=0}^{\rm sr}$  is investigated in [17]. To recall some further results we define the ionization threshold and the ground state energy of  $H_{\gamma}^{\rm sr}$ , respectively, as

$$\Sigma^{\mathrm{sr}} := \inf \sigma[H_0^{\mathrm{sr}}], \qquad E_{\gamma}^{\mathrm{sr}} := \inf \sigma[H_{\gamma}^{\mathrm{sr}}], \quad \gamma \in (0, \gamma_{\mathrm{c}}^{\mathrm{sr}}].$$

Then the following shall be relevant for us:

**Proposition 1.1** ([8, 9]). (i) For all  $e \in \mathbb{R}$ ,  $\Lambda > 0$ , and  $\gamma \in (0, \gamma_{c}^{sr}]$ ,

(1.9) 
$$\Sigma^{\rm sr} - E_{\gamma}^{\rm sr} \ge 1 - \inf \sigma[H_{\gamma}^{\rm el, sr}] > 0$$

(ii) For all  $e \in \mathbb{R}$ ,  $\Lambda > 0$ , and  $\gamma \in (0, \gamma_{c}^{sr})$ ,  $E_{\gamma}^{sr}$  is an eigenvalue of  $H_{\gamma}^{sr}$ .

Proof. Part (i) follows from [8] (at least in the case  $\gamma \in (0, 1/2)$ , where  $H_{\gamma}^{\rm sr}$  is essentially self-adjoint on  $\mathscr{D}$  [10]). An alternative proof of (1.9) covering all  $\gamma \in (0, \gamma_{\rm c}^{\rm sr}]$  can be found in [9]. Part (ii) is the main result of [9].

In the present paper we shall extend the results on the spatial exponential localization of spectral subspaces below  $\Sigma^{\rm sr}$  of  $H_{\gamma}^{\rm sr}$ ,  $\gamma \in (0, \gamma_{\rm c}^{\rm sr})$ , [15] and Proposition 1.1(ii) to the critical case  $\gamma = \gamma_{\rm c}^{\rm sr}$ .

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

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

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

(1.10) 
$$H_{\gamma}^{+} := P_{\mathbf{A}}^{+} \left( D_{\mathbf{A}} + V_{\gamma} + H_{\mathbf{f}} \right) P_{\mathbf{A}}^{+}.$$

Thanks to [15, Proof of Lemma 3.4(ii)], which implies that  $P_{\mathbf{A}}^+$  maps  $\mathscr{D}$  into  $\mathcal{D}(D_{\mathbf{0}}) \cap \mathcal{D}(H_{\mathbf{f}}^{\nu})$ , for every  $\nu > 0$ , and Hardy's inequality, we actually know that  $H_{\gamma}^+$  is well-defined on  $\mathscr{D}$ . Due to [10] the quadratic form associated with  $H_{\gamma}^+$  is semi-bounded below, if and only if  $\gamma$  is less than or equal to

$$\gamma_{\rm c}^{\rm np} := 2/(2/\pi + \pi/2)$$

which is the critical constant in the Brown-Ravenhall model determined in [4]. Again we denote the Friedrichs extension of the no-pair operator by the same symbol  $H_{\gamma}^+$ , if  $\gamma \in [0, \gamma_c^{np}]$ . Because of technical reasons it is convenient to add the following counter-part acting in the negative spectral subspace  $P_{\mathbf{A}}^- \mathscr{H}$ ,

$$H_{\gamma}^{-} := P_{\mathbf{A}}^{-} \left( -D_{\mathbf{A}} + V_{\gamma} + H_{\mathrm{f}} \right) P_{\mathbf{A}}^{-}, \quad \gamma \in \left[ 0, \gamma_{\mathrm{c}}^{\mathrm{np}} \right],$$

which is also defined as a Friedrichs extension starting from  $\mathscr{D}$ . In fact,  $H_{\gamma}^+$ and  $H_{\gamma}^-$  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

(1.11) 
$$H^{\rm np}_{\gamma} := H^+_{\gamma} \oplus H^-_{\gamma} = H^+_{\gamma} \oplus \{\vartheta \ H^+_{\gamma}\vartheta\}.$$

For later reference we observe that

(1.12) 
$$H_{\gamma}^{\rm np} = |D_{\mathbf{A}}| + \frac{1}{2} (V_{\gamma} + H_{\rm f}) + \frac{1}{2} S_{\mathbf{A}} (V_{\gamma} + H_{\rm f}) S_{\mathbf{A}} \quad \text{on } \mathscr{D}.$$

The mathematical analysis of a molecular analogue of  $H^+_{\gamma}$  has been initiated in [12] where the stability of the second kind of relativistic matter has been established in the no-pair model under certain restrictions on e,  $\Lambda$ , and the nuclear charges. Moreover, an upper bound on the (positive) binding energy is derived in [11]. To recall some results on hydrogen-like atoms used later on we put

 $\Sigma^{\mathrm{np}} := \inf \sigma[H_0^{\mathrm{np}}], \qquad E_{\gamma}^{\mathrm{np}} := \inf \sigma[H_{\gamma}^{\mathrm{np}}], \quad \gamma \in (0, \gamma_{\mathrm{c}}^{\mathrm{np}}].$ 

Both parts of the following proposition are proven in [10]:

**Proposition 1.2** ([10]). (i) For all  $e \in \mathbb{R}$ ,  $\Lambda > 0$ , and  $\gamma \in (0, \gamma_c^{np}]$ , there is some  $c(\gamma, e, \Lambda) > 0$  such that

(1.13)  $\Sigma^{\rm np} - E^{\rm np}_{\gamma} \ge c(\gamma, e, \Lambda) \,.$ 

(ii) For all  $e \in \mathbb{R}$ ,  $\Lambda > 0$ , and  $\gamma \in (0, \gamma_{c}^{np})$ ,  $E_{\gamma}^{np}$  is an eigenvalue of  $H_{\gamma}^{np}$ .

The exponential localization of spectral subspaces corresponding to energies below  $\Sigma^{np}$  is shown in [15], again for sub-critical values of  $\gamma$  only. We propose to extend the latter result as well as Proposition 1.2(ii) to the case  $\gamma = \gamma_c^{np}$  in the present article.

We close this subsection by recalling some further results of [10] used later on. In order to improve the localization estimates of [15] and to deal with critical coupling constants the bounds in (1.14) 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 [5, 19] and an analogous inequality for the Brown-Ravenhall model [5].

**Proposition 1.3** ([10]). Let  $\gamma_c$  be  $\gamma_c^{sr}$  or  $\gamma_c^{np}$  and  $H_{\gamma}$  be  $H_{\gamma}^{sr}$  or  $H_{\gamma}^{np}$ . Then, for all  $e \in \mathbb{R}$  and  $\Lambda > 0$ , the following holds:

(i) For  $\gamma \in [0, 1/2)$ ,  $H_{\gamma}$  is essentially self-adjoint on  $\mathscr{D}$ .

(ii) For all  $\varepsilon \in (0, 1)$ ,  $\delta > 0$ , and  $\gamma \in [0, \gamma_{c}]$ ,

(1.14) 
$$|D_{\mathbf{0}}|^{\varepsilon} \leq \delta H_{\gamma} + C(e, \Lambda, \delta, \varepsilon), \qquad |D_{\mathbf{A}}|^{\varepsilon} \leq \delta H_{\gamma} + C'(e, \Lambda, \delta, \varepsilon),$$

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

(*iii*) 
$$\mathcal{D}(H_{\gamma}) \subset \mathcal{D}(H_{\mathrm{f}})$$
 and, for all  $\delta > 0, \gamma \in [0, \gamma_{\mathrm{c}}]$ , and  $\psi \in \mathcal{D}(H_{\gamma})$ ,

(1.15)  $\|H_{\mathbf{f}}\psi\| \leq (1+\delta) \|H_{\gamma}\psi\| + C(e,\Lambda,\delta) \|\psi\|.$ 

# 2. EXPONENTIAL LOCALIZATION

In this section we show that low-lying spectral subspaces of  $H_{\gamma}^{\rm sr}$  and  $H_{\gamma}^{\rm np}$  are exponentially localized with respect to **x** in a  $L^2$  sense. This result is stated and proven in Theorem 2.4 at the end of this section. The general idea behind its proof, which rests on a simple identity involving the spectral projection (see (2.7)) and the Helffer-Sjöstrand formula, is due to [1]. (More precisely, (2.7) is variant of a similar identity used in [1]. It has been employed earlier in [14].) 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 2.3). Moreover, one has to derive a useful resolvent identity involving the comparison operator and the original one (Lemma 2.2). In these steps our arguments are more streamlined and simpler than those used in the earlier paper [15] as we work with a simpler comparison operator. Moreover, we now treat critical  $\gamma$  as well. By now these improvements are possible thanks to the results of [10] collected in Proposition 1.3.

In the whole section we fix some  $\mu \in C_0^{\infty}(\mathbb{R}^3_{\mathbf{x}}, [0, 1])$  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

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

and define two comparison operators (compare (1.12)),

$$\begin{aligned} H_{\gamma,R}^{\rm sr} &:= |D_{\mathbf{A}}| + V_{\gamma,R} + H_{\rm f} \,, \quad \gamma \in (0, \gamma_{\rm c}^{\rm sr}] \,, \\ H_{\gamma,R}^{\rm np} &:= |D_{\mathbf{A}}| + \frac{1}{2} \left( V_{\gamma,R} + H_{\rm f} \right) + \frac{1}{2} S_{\mathbf{A}} \left( V_{\gamma,R} + H_{\rm f} \right) S_{\mathbf{A}} \,, \quad \gamma \in (0, \gamma_{\rm c}^{\rm np}] \,, \end{aligned}$$

on the domain  $\mathscr{D}$  to start with. According to Proposition 1.3(i) both operators then are essentially self-adjoint and we again use the symbols  $H_{\gamma,R}^{\rm sr}$  and  $H_{\gamma,R}^{\rm np}$ to denote their self-adjoint closures. Clearly,

(2.1) 
$$H_{\gamma,R}^{\mathrm{sr}} \ge \Sigma^{\mathrm{sr}} - \|V_{\gamma,R}\|_{\infty}, \qquad H_{\gamma,R}^{\mathrm{np}} \ge \Sigma^{\mathrm{np}} - \|V_{\gamma,R}\|_{\infty},$$

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

(2.2) 
$$\begin{cases} \text{The symbols } H, H_R, \Sigma, E \text{ denote either} \\ H_{\gamma}^{\text{sr}}, H_{\gamma,R}^{\text{sr}}, \Sigma^{\text{sr}}, E_{\gamma}^{\text{sr}} \text{ or } H_{\gamma}^{\text{np}}, H_{\gamma,R}^{\text{np}}, \Sigma^{\text{np}}, E_{\gamma}^{\text{np}}. \end{cases}$$

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  $\chi \in C^{\infty}(\mathbb{R}^3_{\mathbf{x}}, [0, 1])$  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,

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

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

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

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

**Lemma 2.1.** Let  $z \in \mathbb{C} \setminus \mathbb{R}$ ,  $R \ge 1$ ,  $F \in \mathscr{W}_a$ , and  $a \in (0, 1/2]$ . Then  $U_R^F(z)$  and  $W_R^F(z)$  extend to bounded operators on  $\mathscr{H}$  and

$$\sup_{F \in \mathscr{W}_a} \|U_R^F(z)\| \leqslant C(e,\Lambda,R) \frac{1 \vee |\operatorname{Re} z|}{1 \wedge |\operatorname{Im} z|}, \quad \sup_{F \in \mathscr{W}_a} \|W_R^F(z)\| \leqslant C'(e,\Lambda,R) \frac{1 \vee |\operatorname{Re} z|}{1 \wedge |\operatorname{Im} z|}$$

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

$$U_{R}^{F}(z) = \frac{1}{2} S_{\mathbf{A}} (H_{\gamma}^{np} - z)^{-1} (V_{\gamma,R} - V_{\gamma}) e^{F} \left[ e^{-F} S_{\mathbf{A}} e^{F}, \chi_{R} \right] \quad \text{on } \mathscr{D},$$

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

$$\left\| \left| \hat{\mathbf{x}} \right|^{-\kappa} (H_{\mathrm{f}} + 1)^{-1/2} \left[ e^{-F} S_{\mathbf{A}} e^{F}, \chi_{R} \right] \right\| \leq C(e, \Lambda, \kappa) \left\| \nabla \chi \right\| / R$$

for every  $\kappa \in [0, 1)$ . Combining the previous bound with the following consequence of  $|\hat{\mathbf{x}}|^{-1/2} \leq C |D_0|^{1/2}$ , (1.14), and (1.15),

$$\left\| \left\| \hat{\mathbf{x}} \right\|^{-1/8} H_{\mathrm{f}}^{1/2} \psi \right\|^{2} \leq \left\| \left\| \hat{\mathbf{x}} \right\|^{-1/4} \psi \right\| \left\| H_{\mathrm{f}} \psi \right\| \leq C(e, \Lambda) \frac{1 \vee |\operatorname{Re} z|^{2}}{1 \wedge |\operatorname{Im} z|^{2}} \left\| (H_{\gamma}^{\mathrm{np}} - \overline{z}) \psi \right\|^{2},$$

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

$$\begin{split} \left\| U_R^F(z) \,\varphi \right\| &\leqslant \frac{1}{2} \left\| \left| \hat{\mathbf{x}} \right|^{-1/8} \left( H_{\mathrm{f}} + 1 \right)^{1/2} (H_{\gamma}^{\mathrm{np}} - \overline{z})^{-1} \right\| \left\| e^F \mu_R \right\| \\ & \cdot \left\| \left| \hat{\mathbf{x}} \right|^{-7/8} (H_{\mathrm{f}} + 1)^{-1/2} [e^{-F} S_{\mathbf{A}} e^F, \chi_R] \varphi \right\| \\ &\leqslant C'(e, \Lambda) \left( e^{2aR} / R \right) \frac{1 \vee |\operatorname{Re} z|}{1 \wedge |\operatorname{Im} z|} \left\| \varphi \right\|, \qquad \varphi \in \mathscr{D}. \end{split}$$

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

(2.3) 
$$\| [\chi_R, S_\mathbf{A}] e^F \| + \| |D_\mathbf{A}|^{-1/4} [\chi_R, |D_\mathbf{A}|] e^F \| \leq C \| \nabla \chi_R e^F \|_{\infty} \leq C' e^{4aR} / R.$$

Here we also used that  $0 \leq F \leq 4aR$  on  $\operatorname{supp}(\nabla \chi_R)$ . On account of (1.14) we also have

$$\left\| \left| D_{\mathbf{A}} \right|^{1/4} (H_{\gamma}^{\mathrm{sr}} - \overline{z})^{-1} \right\| \leqslant C(e, \Lambda) \frac{1 \vee |\operatorname{Re} z|}{1 \wedge |\operatorname{Im} z|}.$$

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

(2.4)  

$$\begin{bmatrix} \chi_{R} , H_{\gamma,R}^{np} \end{bmatrix} e^{F} = [\chi_{R} , |D_{\mathbf{A}}|] e^{F} \\
+ \frac{1}{2} [\chi_{R}, S_{\mathbf{A}}] e^{F} H_{f} e^{-F} S_{\mathbf{A}} e^{F} + \frac{1}{2} S_{\mathbf{A}} H_{f} [\chi_{R}, S_{\mathbf{A}}] e^{F} \\
+ \frac{1}{2} [\chi_{R}, S_{\mathbf{A}}] e^{F} V_{\gamma,R} e^{-F} S_{\mathbf{A}} e^{F} + \frac{1}{2} S_{\mathbf{A}} V_{\gamma,R} [\chi_{R}, S_{\mathbf{A}}] e^{F}.$$

The first term on the RHS of (2.4) is dealt with exactly as in the case of the SRPF operator above. Moreover, on account of (2.3) and  $||e^{-F}S_{\mathbf{A}}e^{F}|| \leq 1+Ca$  (see (A.7)) the norms of both operators in the third line of (2.4) are bounded by some *F*-independent constant times  $e^{4aR}/R^2$ . By Lemma A.5 we finally have

$$\left\| (H_{\rm f}+1)^{-1} \left[ \chi_R, S_{\rm A} \right] e^F H_{\rm f} \right\| \leq C(e,\Lambda) \| \nabla \chi_R e^F \|_{\infty} \leq C(e,\Lambda) \| \nabla \chi \| e^{4aR} / R,$$

and we conclude by means of the following consequence of (1.15),

$$\left\| H_{\mathrm{f}} S_{\mathbf{A}} \left( H_{\gamma}^{\mathrm{np}} - \overline{z} \right)^{-1} \right\| = \left\| H_{\mathrm{f}} \left( H_{\gamma}^{\mathrm{np}} - \overline{z} \right)^{-1} \right\| \leqslant C(e, \Lambda) \frac{1 \vee |\operatorname{Re} z|}{1 \wedge |\operatorname{Im} z|}.$$

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

**Lemma 2.2.** For all  $z \in \mathbb{C} \setminus \mathbb{R}$ ,  $R \ge 1$ ,  $F \in \mathscr{W}_a$ , and  $a \in (0, \frac{1}{2}]$ ,

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

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

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

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

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

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

**Lemma 2.3.** There exist  $g: (0, \infty) \to (0, \infty)$  and  $a_0 \in (0, 1/2]$  such that the following bound holds, for all  $\delta > 0$  and  $a \in (0, a_0]$ ,

$$\sup\left\{ \left\| e^F (H_R - z)^{-1} e^{-F} \right\| : F \in \mathscr{W}_a, \operatorname{Re} z \leq \Sigma - \| V_{\gamma,R} \|_{\infty} - g(a) - \delta \right\} \leq \frac{1}{\delta}.$$

In the case of the SRPF operator we may choose  $a_0 = 1/2$  and  $g(a) = C a^2$ , for some universal constant C > 0. In the case of the no pair operator we may choose  $g(a) = C(e, \Lambda) a$ .

*Proof.* It suffices to show that, for  $\operatorname{Re} z \leq \Sigma - \|V_{\gamma,R}\|_{\infty} - g(a) - \delta$  and  $\psi \in \mathscr{D}$ ,

(2.5) 
$$\delta \|\psi\|^2 \leq \operatorname{Re} \left\langle \psi \left| e^F (H_R - z) e^{-F} \psi \right\rangle \leq \|\psi\| \left\| e^F (H_R - z) e^{-F} \psi \right\|.$$

In fact, if  $F \in \mathscr{W}_a$ , then  $e^{-F}$  maps  $\mathscr{D}$  bijectively into itself, thus  $(H_R - z) e^{-F} \mathscr{D}$  is dense in  $\mathscr{H}$ , as we know that  $H_R$  is essentially self-adjoint on  $\mathscr{D}$  and  $z \in \varrho(H_R)$ . In particular, we may insert  $\psi := e^F (H_R - z)^{-1} e^{-F} \varphi, \varphi \in \mathscr{H}$ , into (2.5), since  $F \in \mathscr{W}_a$  is bounded, and this yields the assertion.

First, we prove (2.5) for the SRPF operator. To this end we put

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

We know from [15, Lemma 3.5] that  $\|\mathcal{K}_F\| \leq C a$ . (We also re-obtain this bound as a special case of (A.5) below.) By a straightforward computation using  $[D_{\mathbf{A}}, e^F]e^{-F} = -i\boldsymbol{\alpha} \cdot \nabla F$  we then find as in [15]

$$\operatorname{Re}\left[e^{F} H_{\gamma,R}^{\operatorname{sr}} e^{-F} - H_{\gamma,R}^{\operatorname{sr}}\right] = \operatorname{Re}\left[e^{F} |D_{\mathbf{A}}| e^{-F} - |D_{\mathbf{A}}|\right]$$
$$= \frac{1}{2} D_{\mathbf{A}}\left[e^{-F}, \left[S_{\mathbf{A}}, e^{F}\right]\right] - \frac{i}{2} \boldsymbol{\alpha} \cdot \nabla F \left(\mathcal{K}_{F} - \mathcal{K}_{-F}\right) \quad \text{on } \mathscr{D}.$$

On account of  $\|\mathcal{K}_F\| \leq C a$ ,  $\|\boldsymbol{\alpha} \cdot \nabla F\| \leq \|\nabla F\|_{\infty} \leq a$ , and the bound

(2.6) 
$$\left\| D_{\mathbf{A}} \left[ e^{-F}, \left[ S_{\mathbf{A}}, e^{F} \right] \right] \right\| \leqslant C' \left\| \nabla F \right\|_{\infty}^{2} \leqslant C' a^{2}$$

proven in [15, Lemma 3.6] and Lemma A.4 below we arrive at

$$\operatorname{Re}\left[e^{F}H_{\gamma,R}^{\operatorname{sr}}e^{-F}\right] \geqslant H_{\gamma,R}^{\operatorname{sr}} - C''a^{2} \geqslant \Sigma^{\operatorname{sr}} - \|V_{\gamma,R}\|_{\infty} - C''a^{2} \quad \text{on } \mathscr{D}.$$

Therefore, we obtain (2.5) for the SRPF operator.

Next, we treat the no-pair operator. In this case

$$e^{F} H_{\gamma,R}^{\rm np} e^{-F} - H_{\gamma,R}^{\rm np} = e^{F} |D_{\mathbf{A}}| e^{-F} - |D_{\mathbf{A}}| + \frac{1}{2} \triangle(V_{\gamma,R}) + \frac{1}{2} \triangle(H_{\rm f})$$

on  $\mathscr{D}$ , where

 $\Delta(T) := e^F S_{\mathbf{A}} T S_{\mathbf{A}} e^{-F} - S_{\mathbf{A}} T S_{\mathbf{A}} = -S_{\mathbf{A}} T \mathcal{K}_F - \mathcal{K}_F T S_{\mathbf{A}} + \mathcal{K}_F T \mathcal{K}_F,$ for  $T = V_{\gamma,R}$  and  $T = H_{\mathrm{f}}$ . Clearly,  $\|\Delta(V_{\gamma,R})\| \leq \mathcal{O}(a) \|V_{\gamma,R}\|_{\infty}$  since  $\|\mathcal{K}_F\| \leq C a$ , and

$$\begin{aligned} |\langle \varphi | \triangle(H_{\mathrm{f}}) \varphi \rangle| &\leq a \langle \varphi | S_{\mathbf{A}} H_{\mathrm{f}} S_{\mathbf{A}} \varphi \rangle + (1 + 1/a) \left\| H_{\mathrm{f}}^{1/2} \mathcal{K}_{F} \varphi \right\|^{2} \\ &\leq a C(e, \Lambda) \langle \varphi | (H_{\gamma, R}^{\mathrm{np}} + \| V_{\gamma, R} \|_{\infty}) \varphi \rangle, \end{aligned}$$

for all  $a \in (0, 1/2]$  and  $\varphi \in \mathcal{D}$ , where we used

$$\left\| H_{\mathrm{f}}^{1/2} \mathcal{K}_{F} \left( H_{\mathrm{f}} + 1 \right)^{-1/2} \right\| \leq C(e, \Lambda) a$$

in the second step, which follows from (A.12) below. Therefore,

$$\operatorname{Re}\left[e^{F} H_{\gamma,R}^{\operatorname{np}} e^{-F}\right] \geq \left(1 - \mathcal{O}(a)\right) H_{\gamma,R}^{\operatorname{np}} - \mathcal{O}(a) \|V_{\gamma,R}\|_{\infty} - C'' a^{2}$$
$$\geq \Sigma^{\operatorname{np}} - \|V_{\gamma,R}\|_{\infty} - \mathcal{O}(a) \Sigma^{\operatorname{np}},$$

for all sufficiently small a > 0, and we conclude as above in the SRPF case.  $\Box$ 

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

**Theorem 2.4 (Exponential localization).** Let  $e \in \mathbb{R}$  and  $\Lambda > 0$ . Then the following assertions hold true:

(i) There is some universal constant, C > 0, such that, for all  $\lambda < \Sigma^{\mathrm{sr}}$ ,  $a \in (0, \frac{1}{2}]$  with  $\Delta := \Sigma^{\mathrm{sr}} - \lambda - C a^2 > 0$ , and  $\gamma \in (0, \gamma_{\mathrm{c}}^{\mathrm{sr}}]$ , we have  $\operatorname{Ran}(\mathbb{1}_{\lambda}(H_{\gamma}^{\mathrm{sr}})) \subset \mathcal{D}(e^{a|\hat{\mathbf{x}}|})$  and

$$\left\| e^{a|\hat{\mathbf{x}}|} \, \mathbb{1}_{\lambda}(H_{\gamma}^{\mathrm{sr}}) \right\| \leq C(e, \Lambda, \Delta).$$

(ii) There is some  $C(e, \Lambda) > 0$ , such that, for all  $\lambda < \Sigma^{np}$ , a > 0 with  $\Delta := \Sigma^{np} - \lambda - C(e, \Lambda) a > 0$ , and  $\gamma \in (0, \gamma_c^{np}]$ , we have  $\operatorname{Ran}(\mathbb{1}_{\lambda}(H_{\gamma}^{np})) \subset \mathcal{D}(e^{a|\hat{\mathbf{x}}|})$ and

$$\left\| e^{a|\hat{\mathbf{x}}|} \, \mathbb{1}_{\lambda}(H_{\gamma}^{\mathrm{np}}) \right\| \leqslant C'(e,\Lambda,\Delta) \,.$$

*Proof.* We treat both models simultaneously again using the notation (2.2) and the function g appearing in the statement of Lemma 2.3.

We put  $\Delta := \Sigma - \lambda - g(a)$  and choose  $R := 1 \vee (3/\Delta)$  so that  $H_R \ge \Sigma - \|V_R\|_{\infty} \ge \Sigma - \Delta/3$ ; recall (2.1). Then 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

(2.7) 
$$\chi_R \mathbb{1}_{\lambda}(H) = \left(\chi_R f(H) - f(H_R) \chi_R\right) \mathbb{1}_{\lambda}(H).$$

(This identity with  $\chi_R$  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

$$\begin{split} \mathrm{supp}(f) \subset [E-1,\lambda+\Delta/3] + i \, [-1,1] \,, \quad |\partial_{\overline{z}} f(z)| \leqslant C(\Delta,N) \, |\mathrm{Im}\, z|^N, \ z \in \mathbb{C} \,, \\ \text{and apply the Helffer-Sjöstrand formula,} \end{split}$$

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

which is valid, for any self-adjoint operator T in some Hilbert space; see, e.g., [3]. Combining it with (2.7) and Lemma 2.2 we obtain, for every  $F \in \mathcal{W}_a$ ,

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

Applying Lemma 2.1 and Lemma 2.3 (with  $\delta = \Delta/3$ ) we arrive at

$$\sup_{F \in \mathscr{W}_a} \left\| \chi_R e^F \mathbb{1}_{\lambda}(H) \right\| \leqslant \frac{C(e,\Lambda,R)}{\Delta} \int_{\mathbb{C}} \frac{|\partial_{\overline{z}}f(z)|}{|\operatorname{Im} z|} \left| dz \wedge d\overline{z} \right| \leqslant C(e,\Lambda,\Delta) \,.$$

To conclude we pick a sequence  $F_n \in \mathscr{W}_a$ ,  $n \in \mathbb{N}$ , converging monotonically to  $a|\mathbf{x}|-a$  on  $\{|\mathbf{x}| \ge 2\}$ . Then, by monotone convergence,  $\int_{\mathbb{R}^3} e^{2a|\mathbf{x}|} \|\psi(\mathbf{x})\|_{\mathscr{F}^4_b}^2 d^3\mathbf{x} = \lim_{n \to \infty} \int_{\mathbb{R}^3} e^{2F_n(\mathbf{x})} \|\psi(\mathbf{x})\|_{\mathscr{F}^4_b}^2 d^3\mathbf{x} \leqslant C'(e, \Lambda, \Delta)$ , for  $\psi \in \operatorname{Ran}(\mathbb{1}_{\lambda}(H)) \subset \int_{\mathbb{R}^3}^{\oplus} \mathscr{F}^4_b d^3\mathbf{x}$ .

## 3. Ground states at critical coupling

Starting from the assertions of Propositions 1.1(ii) and 1.2(ii), namely that  $H_{\gamma}^{\rm sr}$  and  $H_{\gamma}^{\rm np}$  have eigenvalues at the bottom of their spectra, as long as  $\gamma$  is sub-critical, we prove in this section that both operators still possess ground state eigenvectors, when  $\gamma$  attains the critical values  $\gamma_{\rm c}^{\rm sr}$  and  $\gamma_{\rm c}^{\rm np}$ , respectively.

We shall make use of the following abstract lemma which is a variant of a result we learned from [1]; see [9, Lemma 5.1] for a proof.

**Lemma 3.1.** Let  $T, T_1, T_2, \ldots$  be self-adjoint operators acting in some separable Hilbert space,  $\mathscr{X}$ , 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  $0 \neq \phi \in \mathscr{X}$ , then  $E := \lim_{j\to\infty} E_j$  exists and is an eigenvalue of T. If  $E_j = \inf \sigma[T_j]$ , then T is semibounded below and  $E = \inf \sigma[T]$ .

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

(3.1) 
$$\begin{cases} \text{The symbols } H_{\gamma}, \Sigma, E_{\gamma}, \gamma_{c} \text{ denote either} \\ H_{\gamma}^{sr}, \Sigma^{sr}, E_{\gamma}^{sr}, \gamma_{c}^{sr} \text{ or } H_{\gamma}^{np}, \Sigma^{np}, E_{\gamma}^{np}, \gamma_{c}^{np}. \end{cases}$$

**Lemma 3.2.**  $H_{\gamma}$  converges to  $H_{\gamma_{c}}$  in the strong resolvent sense, as  $\gamma \nearrow \gamma_{c}$ . In particular,

(3.2) 
$$\limsup_{\gamma < \gamma_c} E_{\gamma} \leqslant E_{\gamma_c} \,.$$

Proof. For every  $\gamma \in (0, \gamma_{\rm c})$ , we know that  $\mathcal{Q}(H_{\gamma}) = \mathcal{Q}(|D_{\mathbf{0}}|) \cap \mathcal{Q}(H_{\rm f}) \subset \mathcal{Q}(H_{\gamma_{\rm c}})$ [10]. Since  $\mathscr{D}$  is a form core for  $H_{\gamma_{\rm c}}$  we thus have  $\overline{\cap_{\gamma < \gamma_{\rm c}} \mathcal{Q}(H_{\gamma})} = \mathcal{Q}(H_{\gamma_{\rm c}})$ , where the closure is taken with respect to the form norm of  $H_{\gamma_{\rm c}}$ . Since the expectation values  $\langle \varphi | H_{\gamma} \varphi \rangle \searrow \langle \varphi | H_{\gamma_{\rm c}} \varphi \rangle$  converge monotonically, as  $\gamma \nearrow \gamma_{\rm c}$ , for every  $\varphi \in \cap_{\gamma < \gamma_{\rm c}} \mathcal{Q}(H_{\gamma}) = \mathcal{Q}(|D_{\mathbf{0}}|) \cap \mathcal{Q}(H_{\rm f})$ , it follows from [20, Satz 9.23a] that  $H_{\gamma}$ converges to  $H_{\gamma_{\rm c}}$  in the strong resolvent sense.

In order to verify the assumption  $\phi \neq 0$  of Lemma 3.1 we shall adapt a compactness argument from [7]. 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 [7]. To state these bounds for our models we recall the notation

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

almost everywhere, for  $\psi = (\psi^{(n)})_{n=0}^{\infty} \in \mathscr{F}_{\mathrm{b}}[\mathscr{K}]$ , and  $a(k)(\psi^{(0)}, 0, 0, \dots) = 0$ .

**Proposition 3.3 (Infra-red bounds).** Let  $e \in \mathbb{R}$  and  $\Lambda > 0$ . Then there is some  $C(e, \Lambda) \in (0, \infty)$ , such that, for all  $\gamma \in (0, \gamma_c)$  and every normalized ground state eigenvector,  $\phi_{\gamma}$ , of  $H_{\gamma}$ , we have the soft photon bound,

(3.3) 
$$\|a(k)\phi_{\gamma}\|^{2} \leqslant \mathbb{1}_{\{|\mathbf{k}|\leqslant\Lambda\}} \frac{C(e,\Lambda)}{|\mathbf{k}|},$$

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

(3.4) 
$$\|a(\mathbf{k},\lambda)\phi_{\gamma} - a(\mathbf{p},\lambda)\phi_{\gamma}\| \leq C(e,\Lambda) \|\mathbf{k} - \mathbf{p}\| \left(\frac{1}{|\mathbf{k}|^{1/2}|\mathbf{k}_{\perp}|} + \frac{1}{|\mathbf{p}|^{1/2}|\mathbf{p}_{\perp}|}\right),$$

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 (1.3).) In particular,

(3.5) 
$$\sup_{\gamma \in (0,\gamma_{\rm c})} \sum_{n=1}^{\infty} n \, \|\phi_{\gamma}^{(n)}\|^2 < \infty \,,$$

where  $\phi_{\gamma} = (\phi_{\gamma}^{(n)})_{n=0}^{\infty} \in \bigoplus_{n=0}^{\infty} L^2(\mathbb{R}^3, \mathbb{C}^4) \otimes \mathscr{F}_{\mathrm{b}}^{(n)}[\mathscr{K}].$ 

*Proof.* First, we prove the soft photon bound (3.3) for the SRPF operator. To this end we put

 $R_{\mathbf{A}}(iy) := (D_{\mathbf{A}} - iy)^{-1}, \quad y \in \mathbb{R}, \qquad \mathcal{R}_{\mathbf{k}} := (H_{\gamma}^{\mathrm{sr}} - E_{\gamma}^{\mathrm{sr}} + |\mathbf{k}|)^{-1}, \quad \mathbf{k} \neq 0,$ and (recall (1.5))

$$\widetilde{\mathbf{G}}_{\mathbf{x}}(k) := \mathbf{G}_{\mathbf{x}}(k) - \mathbf{G}_{\mathbf{0}}(k) = \mathbf{G}_{\mathbf{0}}(k) \left( e^{-i\mathbf{k}\cdot\mathbf{x}} - 1 \right).$$

For  $\gamma \in (0, \gamma_{\rm c}^{\rm sr})$ , we derived the following representation in [9],

$$a(k) \phi_{\gamma} := i (|\mathbf{k}| \mathcal{R}_{\mathbf{k}} - 1) \mathbf{G}_{\mathbf{0}}(k) \cdot \hat{\mathbf{x}} \phi_{\gamma} - \mathcal{R}_{\mathbf{k}} \boldsymbol{\alpha} \cdot \widetilde{\mathbf{G}}_{\hat{\mathbf{x}}}(k) S_{\mathbf{A}} \phi_{\gamma} + I_{\gamma}(k) ,$$

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

$$I_{\gamma}(k) := \int_{\mathbb{R}} \mathcal{R}_{\mathbf{k}} D_{\mathbf{A}} R_{\mathbf{A}}(iy) \, \boldsymbol{\alpha} \cdot \widetilde{\mathbf{G}}_{\hat{\mathbf{x}}}(k) \, R_{\mathbf{A}}(iy) \, \phi_{\gamma} \, \frac{dy}{\pi} \, .$$

Here the Bochner integral  $I_{\gamma}(k)$  is actually absolutely convergent. In fact, pick some  $F \in C^{\infty}(\mathbb{R}^3_{\mathbf{x}}, [0, \infty))$  such that  $F(\mathbf{x}) = a|\mathbf{x}|$ , for large  $|\mathbf{x}|$ , and  $|\nabla F| \leq a$ , where a is sufficiently small. By virtue of (1.14) and Theorem 2.4 we then obtain

$$\begin{split} \|I_{\gamma}(k)\| &\leqslant \int_{\mathbb{R}} \left\{ \left\| \left| D_{\mathbf{A}} \right|^{1/4} \mathcal{R}_{\mathbf{k}} \right\| \left\| \left| D_{\mathbf{A}} \right|^{3/4} R_{\mathbf{A}}(iy) \right\| \right. \\ & \left. \cdot \left| \mathbf{G}_{\mathbf{0}}(k) \right| \sup_{\mathbf{x}} \left| \left( e^{-i\mathbf{k}\cdot\mathbf{x}} - 1 \right) e^{-F(\mathbf{x})} \right| \left\| e^{F} R_{\mathbf{A}}(iy) e^{-F} \right\| \left\| e^{F} \phi_{\gamma} \right\| \right\} \frac{dy}{\pi} \,. \end{split}$$

Here  $|||D_{\mathbf{A}}|^{1/4} \mathcal{R}_{\mathbf{k}}|| \leq C(e, \Lambda)/(1 \wedge |\mathbf{k}|)$  by (1.14),  $|||D_{\mathbf{A}}|^{3/4} \mathcal{R}_{\mathbf{A}}(iy)|| \leq C \langle y \rangle^{-1/4}$ , and the composition  $e^F \mathcal{R}_{\mathbf{A}}(iy) e^{-F}$  is well-defined with  $||e^F \mathcal{R}_{\mathbf{A}}(iy) e^{-F}|| \leq C \langle y \rangle^{-1}$  by Lemma A.1 below. Using also  $|\mathbf{G}_{\mathbf{0}}(k)| \leq (|e|/2\pi) |\mathbf{k}|^{-1/2} \mathbb{1}_{\{|\mathbf{k}| \leq \Lambda\}}$ and  $|e^{-i\mathbf{k}\cdot\mathbf{x}} - 1| \leq |\mathbf{k}| |\mathbf{x}|$ , we arrive at the  $\gamma$ -independent estimate

$$\|I_{\gamma}(k)\| \leqslant \mathbb{1}_{\{|\mathbf{k}| \leqslant \Lambda\}} \frac{C'(e,\Lambda) \, |\mathbf{k}|^{1/2}}{1 \wedge |\mathbf{k}|} \cdot \sup_{\gamma < \gamma_c^{\mathrm{sr}}} \|e^F \phi_{\gamma}\| \leqslant \mathbb{1}_{\{|\mathbf{k}| \leqslant \Lambda\}} \frac{C''(e,\Lambda)}{|\mathbf{k}|^{1/2}},$$

for almost every  $k = (\mathbf{k}, \lambda) \in \mathbb{R}^3 \times \mathbb{Z}_2$ . Now, it is also clear how to estimate the remaining terms in the formula for  $a(k) \phi_{\gamma}$  and to get (3.3). (Notice that  $\|e^F S_{\mathbf{A}} \phi_{\gamma}\| \leq \|e^F S_{\mathbf{A}} e^{-F}\| \|e^F \phi_{\gamma}\|$ , where  $\|e^F S_{\mathbf{A}} e^{-F}\| \leq 1 + C a$  by (A.7) and a simple approximation argument.)

In a similar fashion we next derive the photon derivative bound (3.4) for the SRPF operator. In fact,  $\|(\mathcal{R}_{\mathbf{k}} - \mathcal{R}_{\mathbf{p}})\psi\| \leq |\mathbf{p}|^{-1}|\mathbf{k} - \mathbf{p}| \|\mathcal{R}_{\mathbf{k}}\psi\|, \psi \in \mathscr{H}$ , by the first resolvent identity, thus

$$\begin{split} \|I_{\gamma}(\mathbf{k},\lambda) - I_{\gamma}(\mathbf{p},\lambda)\| \\ &\leqslant \int_{\mathbb{R}} \left\{ \left\| \left| D_{\mathbf{A}} \right|^{1/4} \mathcal{R}_{\mathbf{k}} \right\| \left\| \left| D_{\mathbf{A}} \right|^{3/4} R_{\mathbf{A}}(iy) \right\| \\ &\cdot \sup_{\mathbf{x}} \left\{ |\widetilde{\mathbf{G}}_{\mathbf{x}}(\mathbf{k},\lambda) - \widetilde{\mathbf{G}}_{\mathbf{x}}(\mathbf{p},\lambda)| e^{-F(\mathbf{x})} \right\} \| e^{F} R_{\mathbf{A}}(iy) e^{-F} \| \| e^{F} \phi_{\gamma} \| \right\} \frac{dy}{\pi} \\ &+ \frac{|\mathbf{k} - \mathbf{p}|}{|\mathbf{p}|} \int_{\mathbb{R}} \left\{ \left\| \left| D_{\mathbf{A}} \right|^{1/4} \mathcal{R}_{\mathbf{k}} \right\| \| \left| D_{\mathbf{A}} \right|^{3/4} R_{\mathbf{A}}(iy) \right\| \\ &\cdot \sup_{\mathbf{x}} \left\{ |\widetilde{\mathbf{G}}_{\mathbf{x}}(\mathbf{p},\lambda)| e^{-F(\mathbf{x})} \right\} \| e^{F} R_{\mathbf{A}}(iy) e^{-F} \| \| e^{F} \phi_{\gamma} \| \right\} \frac{dy}{\pi} \,. \end{split}$$

Here  $|\widetilde{\mathbf{G}}_{\mathbf{x}}(\mathbf{p}, \lambda)| \leq (|e|/2\pi) |\mathbf{p}|^{1/2} |\mathbf{x}| \mathbb{1}_{\{|\mathbf{p}| \leq \Lambda\}}$  and some elementary estimates [7] (see also [9, §6.3]) using the special choice (1.4) of the polarization vectors reveal that

(3.6) 
$$\frac{|\widetilde{\mathbf{G}}_{\mathbf{x}}(\mathbf{k},\lambda) - \widetilde{\mathbf{G}}_{\mathbf{x}}(\mathbf{p},\lambda)|}{|\mathbf{k}|} \leqslant C \left(1 + |\mathbf{x}|\right) |\mathbf{k} - \mathbf{p}| \left(\frac{1}{|\mathbf{k}|^{1/2}|\mathbf{k}_{\perp}|} + \frac{1}{|\mathbf{p}|^{1/2}|\mathbf{p}_{\perp}|}\right),$$

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 (3.6). 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 (3.4), 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  $|\mathbf{k}|^{-1} ||\mathbf{k}| \mathbf{G}_{\mathbf{0}}(\mathbf{k}, \lambda) - |\mathbf{p}| \mathbf{G}_{\mathbf{0}}(\mathbf{k}, \lambda)|$  can bounded by the RHS of (3.6), too; see [7] or [9, §6.3].

Finally, in the case of the no-pair operator we already observed in [10, Remark 7.2] that the bound proven in Theorem 2.4(ii) provides a proof of the infra-red bounds (3.3) and (3.4) with a  $\gamma$ -independent constant. In fact, in [10] we derived a formula for  $a(k) \phi_{\gamma}$ , when  $\phi_{\gamma}$  is a ground state eigenvector of  $H_{\gamma}^{\text{np}}, \gamma \in (0, \gamma_{\text{c}})$ , 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 3.4 (Ground states at critical coupling).** For  $e \in \mathbb{R}$  and  $\Lambda > 0$ , the minima of the spectra of both  $H_{\gamma_{\alpha}^{sr}}^{sr}$  and  $H_{\gamma_{\alpha}^{np}}^{+}$  are eigenvalues.

*Proof.* Again we treat both models simultaneously using the notation (3.1). (Recall that in view of (1.11) it suffices to show the existence of ground states for  $H_{\gamma_{n}^{np}}^{np}$  instead of  $H_{\gamma_{n}^{np}}^{+}$  in the no-pair model.)

Let  $\phi_{\gamma}$  denote a normalized ground state eigenvector of  $H_{\gamma}$ , for every  $\gamma \in (0, \gamma_{\rm c})$ . Then the family  $\{\phi_{\gamma}\}_{\gamma \in (0, \gamma_{\rm c})}$  contains some weakly convergent sequence,  $\{\phi_{\gamma_j}\}_{j \in \mathbb{N}}, \gamma_j \nearrow \gamma_{\rm c}$ . We denote the weak limit of the latter by  $\phi_{\gamma_{\rm c}}$ . On account of Lemmata 3.1 and 3.2 it suffices to show that  $\phi_{\gamma_{\rm c}} \neq 0$ .

With the exponential localization and infra-red bounds at hand the following compactness argument is the same as in [7] (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 derivaties w.r.t.  $\mathbf{x}$  [9, 10]. The variant of the argument below can also be used to simplify the proofs in [9, 10].)

Let  $\varepsilon > 0$ . On account of (3.5) we find some  $n_0 \in \mathbb{N}$  such that

(3.7) 
$$\forall \gamma \in (0, \gamma_{c}) : \sum_{n=n_{0}+1}^{\infty} \|\phi_{\gamma}^{(n)}\|^{2} < \frac{\varepsilon}{2}.$$

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

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

and denote the partial Fourier transform of  $\phi_{\gamma,\underline{\theta}}^{(n)}$  with respect to  $\mathbf{x}$  as  $\hat{\phi}_{\gamma,\underline{\theta}}^{(n)}$ . Then the soft photon bound (3.3) shows that  $\hat{\phi}_{\gamma,\underline{\theta}}^{(n)}(\boldsymbol{\xi}, \mathbf{k}_1, \dots, \mathbf{k}_n) = 0$ , for almost every  $(\boldsymbol{\xi}, \mathbf{k}_1, \dots, \mathbf{k}_n) \in \mathbb{R}^{3(n+1)}$ , such that  $|\mathbf{k}_j| > \Lambda$ , for some  $j \in \{1, \dots, n\}$ . Moreover, pick some  $s \in (0, 1)$ . By virtue of (1.14) we then have, for all  $\gamma \in (0, \gamma_c)$ ,  $n \in \mathbb{N}$ , and every choice of  $\underline{\theta}$ ,

$$R^{s} \int_{|\boldsymbol{\xi}| \ge R} \|\hat{\phi}_{\gamma,\underline{\theta}}^{(n)}(\boldsymbol{\xi},\cdot)\|_{L^{2}(\mathbb{R}^{3n})}^{2} d^{3}\boldsymbol{\xi} \leqslant \langle \phi_{\gamma,\underline{\theta}}^{(n)} | (-\Delta)^{s/2} \phi_{\gamma,\underline{\theta}}^{(n)} \rangle$$
  
$$\leqslant \langle \phi_{\gamma} | H_{\gamma} \phi_{\gamma} \rangle + C(e,\Lambda,s) = E_{\gamma} + C(e,\Lambda,s) \leqslant |E_{\gamma_{c}}| + \Sigma + C(e,\Lambda,s) .$$

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

(3.8) 
$$\sum_{n=1}^{n_0} \left\| \mathbb{1}_{\{|\boldsymbol{\xi}| \ge R\}} \hat{\phi}_{\gamma}^{(n)} \right\|^2 < \frac{\varepsilon}{2}.$$

As in [7] an application of Hölder's inequality with respect to  $d^3 \boldsymbol{\xi} d^{3(n-1)} \mathbf{K}$  and the photon derivative bound (3.4) yield, for  $p \in [1, 2)$  and  $\gamma \in (0, \gamma_c)$ ,

$$\begin{split} \int \int \int \left| \hat{\phi}_{\gamma,\underline{\theta}}^{(n)}(\boldsymbol{\xi},\mathbf{k}+\mathbf{h},\mathbf{K}) - \hat{\phi}_{\gamma,\underline{\theta}}^{(n)}(\boldsymbol{\xi},\mathbf{k},\mathbf{K}) \right|^{p} d^{3}\boldsymbol{\xi} \, d^{3(n-1)}\mathbf{K} \, d^{3}\mathbf{k} \\ &\leqslant C \sum_{\lambda \in \mathbb{Z}_{2}} \int \limits_{\substack{|\mathbf{k}| < \Lambda, \\ |\mathbf{k}+\mathbf{h}| < \Lambda}} \left\| a(\mathbf{k}+\mathbf{h},\lambda) \, \phi_{\gamma} - a(\mathbf{k},\lambda) \, \phi_{\gamma} \, \right\|^{p} d^{3}\mathbf{k} \\ &\leqslant C' \, |\mathbf{h}|^{p} \int \limits_{|(u,v)| < \Lambda} \left\{ \int \limits_{0}^{|(u,v)|} \frac{dr}{|(u,v)|^{p/2}} + \int \limits_{|(u,v)|}^{\Lambda} \frac{dr}{r^{p/2}} \right\} \frac{du \, dv}{|(u,v)|^{p}} = C'' \, |\mathbf{h}|^{p}, \end{split}$$

where the constants  $C, C', C'' \in (0, \infty)$  depend on  $p, n, \Lambda$ , but not on  $\gamma \in (0, \gamma_c)$ . Since  $\phi_{\gamma}^{(n)}$  is permutation symmetric with respect to the variables  $k_1, \ldots, k_n$  the previous estimate implies [18, §4.8] that the weak first order partial derivatives of  $\hat{\phi}_{\gamma,\underline{\theta}}^{(n)}$  with respect to its last 3n variables exist on  $Q_n := B_R \times B_{\Lambda}^n$ , where  $B_{\rho}$  denotes the open ball in  $\mathbb{R}^3$  of radius  $\rho$  centered at the origin, and that

$$\sup_{\gamma \in (0,\gamma_c)} \|\nabla_{\mathbf{k}_i} \hat{\phi}_{\gamma,\underline{\theta}}^{(n)}\|_{L^p(Q_n)} < \infty, \quad p \in [1,2), \quad i = 1, \dots, n, \quad n = 1, \dots, n_0.$$

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

$$\begin{split} \|\nabla_{\boldsymbol{\xi}} \hat{\phi}_{\boldsymbol{\gamma},\underline{\theta}}^{(n)}\|_{L^{p}(Q_{n})} &\leqslant C(p,n,R,\Lambda) \|\nabla_{\boldsymbol{\xi}} \hat{\phi}_{\boldsymbol{\gamma},\underline{\theta}}^{(n)}\|_{L^{2}(\mathbb{R}^{3(n+1)})} \\ &= C'(p,n,R,\Lambda) \|\hat{\mathbf{x}} \, \phi_{\boldsymbol{\gamma},\underline{\theta}}^{(n)}\|_{L^{2}(\mathbb{R}^{3(n+1)})} \leqslant C''(p,n,R,\Lambda) \,. \end{split}$$

As observed in [7] 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  $2 < \frac{3(n_0+1)p}{3(n_0+1)-p}$ , then, for every  $n = 1, \ldots, n_0$  and every choice of  $\underline{\theta}$ , we may apply the Rellich-Kondrashov theorem to show that every subsequence of  $\{\hat{\phi}_{\gamma_j,\underline{\theta}}^{(n)}\}_{j\in\mathbb{N}}$  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  $\{\hat{\phi}_{\gamma_j,\underline{\theta}}^{(n)}\}_{j\in\mathbb{N}}$  converges strongly in  $L^2(Q_n)$  to  $\hat{\phi}_{\gamma_c,\underline{\theta}}^{(n)}$ , for all  $n = 0, \ldots, n_0$  and  $\underline{\theta}$ . Taking (3.7) and (3.8) into account we arrive at

$$\|\phi_{\gamma_{\rm c}}\|^2 = \sum_{n=0}^{\infty} \|\hat{\phi}_{\gamma_{\rm c}}^{(n)}\|^2 \ge \lim_{j \to \infty} \sum_{n=0}^{n_0} \sum_{\underline{\theta}} \|\hat{\phi}_{\gamma_j,\underline{\theta}}^{(n)}\|_{L^2(Q_n)}^2 \ge \lim_{j \to \infty} \|\phi_{\gamma_j}\|^2 - \varepsilon = 1 - \varepsilon.$$

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 [15]. 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,

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

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 [14] for classical vector potentials works for quantized ones without any changes.

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

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

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

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) 
$$S_{\mathbf{A}}\psi = \lim_{\tau \to \infty} \int_{-\tau}^{\tau} R_{\mathbf{A}}(iy) \,\psi \,\frac{dy}{\pi} \,, \qquad \psi \in \mathscr{H}.$$

**Lemma A.2.** For every bounded  $F \in C^{\infty}(\mathbb{R}^3_{\mathbf{x}}, \mathbb{R})$  with  $|\nabla F| \leq 1/2$ , all  $\chi \in C^{\infty}(\mathbb{R}^3_{\mathbf{x}}, [0, 1])$ , and  $\kappa \in [0, 1)$ ,

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

*Proof.* To begin with we put  $\check{H}_{\rm f} := H_{\rm f} + 1$  and observe that

(A.4) 
$$\check{H}_{\rm f}^{-1/2} R_{\rm A}^F(iy) = R_{\rm 0}(iy) \left(\check{H}_{\rm f}^{-1/2} - T R_{\rm A}^F(iy)\right),$$

where  $T \in \mathscr{L}(\mathscr{H})$  is the closure of  $\check{H}_{\mathrm{f}}^{-1/2} \boldsymbol{\alpha} \cdot (\mathbf{A} + i\nabla F)$  and satisfies  $||T|| \leq C(e, \Lambda)$ . In fact, since  $R_{\mathbf{0}}(iy)$  and  $\check{H}_{\mathrm{f}}^{-1/2}$  commute we obtain, for every  $\varphi \in \mathscr{D}$ ,

$$\begin{split} \left\{ \check{H}_{\rm f}^{-1/2} R_{\rm A}^{F}(iy) - R_{\rm 0}(iy) \,\check{H}_{\rm f}^{-1/2} \right\} \left( D_{\rm A} + i\boldsymbol{\alpha}\cdot\nabla F - iy \right) \varphi \\ &= -R_{\rm 0}(iy) \,\check{H}_{\rm f}^{-1/2} \boldsymbol{\alpha} \cdot \left( {\rm A} + i\nabla F \right) \varphi \\ &= -R_{\rm 0}(iy) \,T \, R_{\rm A}^{F}(iy) \left( D_{\rm A} + i\boldsymbol{\alpha}\cdot\nabla F - iy \right) \varphi \,. \end{split}$$

As  $D_{\mathbf{A}}$  is essentially self-adjoint on  $\mathscr{D}$  we know that  $(D_{\mathbf{A}} + i\boldsymbol{\alpha} \cdot \nabla F - iy) \mathscr{D}$  is dense in  $\mathscr{H}$  and we obtain (A.4). (In fact, if  $\psi \in \mathscr{H}$  and  $\varphi_n \in \mathscr{D}$  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,  $|\hat{\mathbf{x}}|^{-2\kappa} \leq C(\kappa) |D_{\mathbf{0}}|^{2\kappa}$ , and  $|| |D_{\mathbf{0}}|^{\kappa} R_{\mathbf{0}}(iy)|| \leq C'(\kappa) \langle y \rangle^{\kappa-1}$  we deduce from (A.2) and (A.4) that

$$\left\| \left| \hat{\mathbf{x}} \right|^{-\kappa} \check{H}_{\mathrm{f}}^{-1/2} R_{\mathbf{A}}^{F}(iy) \right\| \leqslant C''(e,\Lambda,\kappa) \left\langle y \right\rangle^{\kappa-1}.$$

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

$$\begin{split} \left| \left\langle \, | \hat{\mathbf{x}} |^{-\kappa} \, \varphi \, \left| \, \check{H}_{\mathrm{f}}^{-1/2} \left[ e^{F} \, S_{\mathbf{A}} \, e^{-F}, \, \chi \right] \psi \, \right\rangle \right| \\ & \leqslant \int_{\mathbb{R}} \left| \left\langle \, | \hat{\mathbf{x}} |^{-\kappa} \, \varphi \, \left| \, \check{H}_{\mathrm{f}}^{-1/2} \, R_{\mathbf{A}}^{F}(iy) \, i \mathbf{\alpha} \cdot \nabla \chi \, R_{\mathbf{A}}^{F}(iy) \, \psi \, \right\rangle \right| \frac{dy}{\pi} \\ & \leqslant C'''(e, \Lambda, \kappa) \int_{\mathbb{R}} \langle y \rangle^{\kappa - 2} dy \cdot \| \nabla \chi \|_{\infty} \, \| \varphi \| \, \| \psi \| \, , \end{split}$$

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

The bounds derived in the following lemma are slightly more general than the corresponding ones of [15, Lemma 3.5].

**Lemma A.3.** Let  $\kappa \in [0, 1)$ ,  $\varepsilon > 0$ , and  $\chi \in C^{\infty}(\mathbb{R}^3_{\mathbf{x}}, [0, 1])$  with  $|\nabla \chi|$  bounded. Moreover, let  $F, G \in C^{\infty}(\mathbb{R}^3_{\mathbf{x}}, \mathbb{R})$  be bounded with bounded first order derivatives and such that  $|\nabla(F - G)| \leq 1/2$ . Then

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

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

In particular, we have, for every bounded  $G \in C^{\infty}(\mathbb{R}^3_{\mathbf{x}}, \mathbb{R})$  such that  $|\nabla G| \leq 1/2$ ,

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

*Proof.* Combining (A.3), the computation

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

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

$$\begin{aligned} \left| \left\langle \left| D_{\mathbf{A}} \right|^{\kappa} \varphi \right| \left[ \chi e^{G}, S_{\mathbf{A}} \right] e^{F-G} \psi \right\rangle \right| \\ & \leq \int_{\mathbb{R}} \left| \left\langle \left| D_{\mathbf{A}} \right|^{\kappa} \varphi \right| R_{\mathbf{A}}(iy) \, i \boldsymbol{\alpha} \cdot \left( \nabla \chi + \chi \, \nabla G \right) e^{F} \, R_{\mathbf{A}}^{G-F}(iy) \, \psi \right\rangle \right| \frac{dy}{\pi} \end{aligned}$$

$$(A.9) \qquad \leq C''(\kappa) \, \| \left( \nabla \chi + \chi \, \nabla G \right) e^{F} \|_{\infty} \int_{\mathbb{R}} \langle y \rangle^{\kappa-2} dy \, \|\varphi\| \, \|\psi\| \, , \end{aligned}$$

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

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

To derive (A.6) we write  $|D_{\mathbf{A}}| = D_{\mathbf{A}} S_{\mathbf{A}}$  and compute  $[\chi e^{G}, |D_{\mathbf{A}}|] e^{F-G} = i \boldsymbol{\alpha} \cdot (\nabla \chi + \chi \nabla G) e^{F} (e^{G-F} S_{\mathbf{A}} e^{F-G}) + D_{\mathbf{A}} [\chi e^{G}, S_{\mathbf{A}}] e^{F-G}$ on  $\mathscr{D}$ . (Thanks to [15, Proof of Lemma 3.4(ii)] we know that  $S_{\mathbf{A}}$  maps  $e^{F-G} \mathscr{D} = \mathscr{D}$  into  $\mathcal{D}(D_{\mathbf{0}}) \cap \mathcal{D}(H_{\mathbf{f}})$  which is left invariant under multiplication with  $\chi e^{G}$ .) 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 is just a special case of [15, Lemma 3.6].

**Lemma A.4.** For all bounded  $F \in C^{\infty}(\mathbb{R}^3_{\mathbf{x}}, \mathbb{R})$  such that  $|\nabla F| \leq a \leq 1/2$ , the bound (2.6) holds true.

Proof. A straightforward computation yields  $\begin{bmatrix} e^{-F}, [R_{\mathbf{A}}(iy), e^{F}] \end{bmatrix} = R_{\mathbf{A}}(iy) i\boldsymbol{\alpha} \cdot \nabla F \left\{ R_{\mathbf{A}}^{F}(iy) + R_{\mathbf{A}}^{-F}(iy) \right\} i\boldsymbol{\alpha} \cdot \nabla F R_{\mathbf{A}}(iy) .$ Together with (A.2) and (A.3) this permits to get  $\begin{bmatrix} \langle D_{\mathbf{A}} | \varphi | [e^{-F}, [S_{\mathbf{A}} | e^{F}] ] \psi \rangle \end{bmatrix}$ 

$$\| \langle D_{\mathbf{A}} \varphi \| [e^{-y}, [J_{\mathbf{A}}, e^{-y}]] \psi \rangle \|$$

$$\leq \int_{\mathbb{R}} \| D_{\mathbf{A}} R_{\mathbf{A}}(iy) \| \| \nabla F \|_{\infty}^{2} \left( \| R_{\mathbf{A}}^{F}(iy) \| + \| R_{\mathbf{A}}^{-F}(iy) \| \right) \| R_{\mathbf{A}}(iy) \| \frac{dy}{\pi}$$

$$\leq C \| \nabla F \|_{\infty}^{2} \int_{\mathbb{R}} \frac{dy}{\langle y \rangle^{2}},$$

for all normalized  $\varphi \in \mathcal{D}(D_{\mathbf{A}})$  and  $\psi \in \mathscr{H}$ .

The last lemma of this appendix again presents a variant of a bound obtained in [15, Lemma 3.5]. In order to prove it we recall some technical tool introduced in [15]. First, we put

(A.10) 
$$\check{H}_{\mathrm{f}} := H_{\mathrm{f}} + K, \qquad T_{\nu} := [\check{H}_{\mathrm{f}}^{-\nu}, \boldsymbol{\alpha} \cdot \mathbf{A}] \check{H}_{\mathrm{f}}^{\nu} \text{ on } \mathscr{D},$$

and recall the bound  $||T_{\nu}|| \leq C(e, \Lambda)/K^{1/2}$ , for  $\nu \geq 1/2$  and  $K \geq 1$ ; see [15, Lemma 3.1]. In view of (A.2) it shows that, for a sufficiently large choice of  $K \geq 1$ , the Neumann series  $\Xi_{\nu}^{F}(y) := \sum_{\ell=0}^{\infty} \{-R_{\mathbf{A}}^{F}(iy) \overline{T}_{\nu}\}^{\ell}$  converges and

satisfies, say,  $\|\Xi_{\nu}^{F}(y)\| \leq 2$ , for all  $\nu \geq 1/2$ ,  $y \in \mathbb{R}$ , and  $F \in C^{\infty}(\mathbb{R}^{3}_{\mathbf{x}}, \mathbb{R})$  with  $|\nabla F| \leq 1/2$ . Moreover, it is easy to verify the following useful intertwining relation [15, Corollary 3.1],

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

**Lemma A.5.** Let  $\nu \ge 1/2$  and  $\chi$ , F, and G be as in Lemma A.3. Then

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

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

for all normalized  $\varphi, \psi \in \mathscr{D}$ . This implies (A.12) since  $\|(H_{\rm f}+1)^{-\nu}\check{H}_{\rm f}^{\nu}\| \leq K^{\nu}$ , where our choice of K depends only on e and  $\Lambda$ .

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MARTIN KÖNENBERG, FAKULTÄT FÜR MATHEMATIK UND INFORMATIK, FERNUNIVER-SITÄT HAGEN, LÜTZOWSTRASSE 125, D-58084 HAGEN, GERMANY, Present address: FA-KULTÄT FÜR PHYSIK, UNIVERSITÄT WIEN, BOLTZMANNGASSE 5, 1090 VIENNA, AUSTRIA. E-mail address: martin.koenenberg@univie.ac.at

OLIVER MATTE, FAKULTÄT FÜR MATHEMATIK, TU MÜNCHEN, BOLTZMANNSTRASSE 3, D-85748 GARCHING, GERMANY, *Present address:* MATHEMATISCHES INSTITUT, LUDWIG-MAXIMILIANS-UNIVERSITÄT, THERESIENSTRASSE 39, D-80333 MÜNCHEN, GERMANY. *E-mail address:* matte@math.lmu.de