

LOCALIZATION OF THE ESSENTIAL SPECTRUM  
FOR RELATIVISTIC  $N$ -ELECTRON IONS AND ATOMS

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ABSTRACT. The HVZ theorem is proven for the pseudorelativistic  $N$ -electron Jansen-Hess operator ( $2 \leq N \leq Z$ ) which acts on the spinor Hilbert space  $\mathcal{A}(H_1(\mathbb{R}^3) \otimes \mathbb{C}^4)^N$  where  $\mathcal{A}$  denotes antisymmetrization with respect to particle exchange. This 'no pair' operator results from the decoupling of the electron and positron degrees of freedom up to second order in the central potential strength  $\gamma = Ze^2$ .

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INTRODUCTION

We consider  $N$  interacting electrons in a central Coulomb field generated by a point nucleus of charge number  $Z$  which is infinitely heavy and located at the origin. For stationary electrons where the radiation field and pair creation can be neglected, the  $N + 1$  particle system is described by the Coulomb-Dirac operator, introduced by Sucher [23]. The Jansen-Hess operator used in the present work, which acts on the positive spectral subspace of  $N$  free electrons, is derived from the Coulomb-Dirac operator by applying a unitary transformation scheme [12, 13] which is equivalent to the Douglas-Kroll transformation scheme [6]. The transformed operator is represented as an infinite series of operators which do not couple the electron and positron degrees of freedom. For  $N = 1$ , each successive term in this series is of increasing order in the strength  $\gamma$  of the central field. The series has been shown to be convergent for subcritical potential strength ( $\gamma < \gamma_c = 0.3775$ , corresponding to  $Z < 52$  [21]). For  $N > 1$  the expansion parameter is  $e^2$ , which comprises the central field strength  $Ze^2$  and the strength  $e^2$  of the electron-electron interaction. A numerical investigation of the cases  $N = 1$ ,  $Z - 1$  and  $Z$  across the periodic table has revealed [27] that the ground-state energy of an  $N$ -electron system is

already quite well represented if the series is truncated after the second-order term. This approximation defines the Jansen-Hess operator (see (3.1) below). In the present work we provide the localization of the essential spectrum of this operator. Recently [14] we have proven the HVZ theorem (which dates back to Hunziker [10], van Winter [26] and Zhislin [28] for the Schrödinger operator and to Lewis, Siedentop and Vugalter [16] for the scalar pseudorelativistic Hamiltonian) for the two-particle Brown-Ravenhall operator [2] which is the first-order term in the above mentioned series of operators. Now we extend this proof successively to the multiparticle Brown-Ravenhall operator (section 1), to the two-electron Jansen-Hess operator (section 2) and finally to the  $N$ -electron Jansen-Hess operator. We closely follow the earlier work [14] where the details can be found. A quite different proof of the HVZ theorem for the multiparticle Brown-Ravenhall operator is presently under investigation [18].

## 1 MULTIPARTICLE BROWN-RAVENHALL CASE

For  $N$  electrons of mass  $m$  in a central field, generated by a point nucleus which is infinitely heavy and fixed at the origin, the Brown-Ravenhall operator is given by (in relativistic units,  $\hbar = c = 1$ )

$$H^{BR} = \Lambda_{+,N} \left( \sum_{k=1}^N (D_0^{(k)} + V^{(k)}) + \sum_{k>l=1}^N V^{(kl)} \right) \Lambda_{+,N} \quad (1.1)$$

where  $D_0^{(k)} = \boldsymbol{\alpha}^{(k)} \mathbf{p}_k + \beta^{(k)} m$  is the free Dirac operator of electron  $k$ ,  $V^{(k)} = -\gamma/x_k$  is the central potential with strength  $\gamma = Ze^2$ , and  $V^{(kl)} = e^2/|\mathbf{x}_k - \mathbf{x}_l|$  is the electron-electron interaction,  $e^2 \approx 1/137.04$  being the fine structure constant and  $x_k = |\mathbf{x}_k|$  the distance of electron  $k$  from the origin. Further,  $\Lambda_{+,N} = \Lambda_+^{(1)} \cdots \Lambda_+^{(N)}$  (as shorthand for  $\bigotimes_{k=1}^N \Lambda_+^{(k)}$ ) is the (tensor) product of the single-particle projectors  $\Lambda_+^{(k)} = \frac{1}{2}(1 + D_0^{(k)}/E_{p_k})$  onto the positive spectral subspace of  $D_0^{(k)}$ .  $H^{BR}$  acts in the Hilbert space  $\mathcal{A}(L_2(\mathbb{R}^3) \otimes \mathbb{C}^4)^N$ , and is well-defined in the form sense and positive on  $\mathcal{A}(H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^4)^N$  for  $\gamma < \gamma_{BR} = \frac{2}{\pi/2+2/\pi} \approx 0.906$  (see (1.10) below). For the multi-nucleus case the Brown-Ravenhall operator was shown to be positive if  $\gamma < 0.65$  [9].

An equivalent operator, which is defined in a reduced spinor space by means of  $(\psi_+, H^{BR} \psi_+) = (\varphi, h^{BR} \varphi)$  with  $\psi_+ \in \Lambda_{+,N}(\mathcal{A}(H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^4)^N)$  and  $\varphi \in \mathcal{A}(H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^2)^N$ , is [7]

$$h^{BR} = \sum_{k=1}^N (T^{(k)} + b_{1m}^{(k)}) + \sum_{k>l=1}^N v^{(kl)}. \quad (1.2)$$

Explicitly, with  $A_k := A(p_k) = \left( \frac{E_{p_k} + m}{2E_{p_k}} \right)^{1/2}$  and  $G_k := \boldsymbol{\sigma}^{(k)} \mathbf{p}_k g(p_k)$ ,

$g(p_k) = (2E_{p_k}(E_{p_k} + m))^{-1/2}$ , one has [14]

$$\begin{aligned}
 T^{(k)} &:= E_{p_k} = \sqrt{p_k^2 + m^2}, & b_{1m}^{(k)} &= -\gamma \left( A_k \frac{1}{x_k} A_k + G_k \frac{1}{x_k} G_k \right) \\
 v^{(kl)} &= A_k A_l \frac{e^2}{|\mathbf{x}_k - \mathbf{x}_l|} A_k A_l + A_k G_l \frac{e^2}{|\mathbf{x}_k - \mathbf{x}_l|} A_k G_l \\
 &+ G_k A_l \frac{e^2}{|\mathbf{x}_k - \mathbf{x}_l|} G_k A_l + G_k G_l \frac{e^2}{|\mathbf{x}_k - \mathbf{x}_l|} G_k G_l.
 \end{aligned} \tag{1.3}$$

Let us consider the two-cluster decompositions  $\{C_{1j}, C_{2j}\}$  of the  $N$ -electron atom, obtained by moving electron  $j$  far away from the atom or by separating the nucleus from all electrons. Denote by  $C_{1j}$  the cluster located near the origin (containing the nucleus), while  $C_{2j}$  contains either one electron ( $j = 1, \dots, N$ ) or all electrons ( $j = 0$ ). Correspondingly,  $h^{BR}$  is split into

$$h^{BR} = T + a_j + r_j, \quad j = 0, 1, \dots, N, \tag{1.4}$$

with  $T := \sum_{k=1}^N T^{(k)}$ , while  $a_j$  denotes the interaction of the particles located all in cluster  $C_{1j}$  or all in  $C_{2j}$ . The remainder  $r_j$  collects the interactions between particles sitting in different clusters and is supposed to vanish when  $C_{2j}$  is moved to infinity.

Define for  $j \in \{0, 1, \dots, N\}$

$$\Sigma_0 := \min_j \inf \sigma(T + a_j). \tag{1.5}$$

Then we have

**THEOREM 1 (HVZ THEOREM FOR THE MULTIPARTICLE BROWN-RAVENHALL OPERATOR).**

Let  $h^{BR}$  be the Brown-Ravenhall operator for  $N > 2$  electrons in a central field of strength  $\gamma < \gamma_{BR} = \frac{2}{\pi/2+2/\pi}$ , and let (1.4) be its two-cluster decompositions. Then the essential spectrum of  $h^{BR}$  is given by

$$\sigma_{ess}(h^{BR}) = [\Sigma_0, \infty). \tag{1.6}$$

In fact, the assertion (1.6) holds even in a more general case. For  $K \geq 2$  introduce  $K$ -cluster decompositions  $d := \{C_1, \dots, C_K\}$  of the  $N + 1$  particles, and split  $h^{BR} = T + a_d + r_d$  accordingly (where  $T + a_d$  describes the infinitely separated clusters while  $r_d$  comprises all interactions between particles sitting in two different clusters). Let

$$\Sigma_1 := \min_{\#d \geq 2} \inf \sigma(T + a_d). \tag{1.7}$$

Then  $\sigma_{ess}(h^{BR}) = [\Sigma_1, \infty)$  with  $\Sigma_1 = \Sigma_0$ . This result, known from the Schrödinger case [20, p.122], relies on the fact that the electron-electron interaction is repulsive ( $V^{(kl)} \geq 0$  respective  $v^{(kl)} \geq 0$ ) and can be proved as follows.

First consider  $K$ -cluster decompositions of the form  $\#C_1 = N + 1 - (K - 1)$  and  $\#C_i = 1$ ,  $i = 2, \dots, K$  (i.e. one ion and  $K - 1$  separated electrons). For any  $j \in \{1, \dots, N\}$  we use for the two-cluster decompositions the notation  $T + a_j = h_{N-1}^{BR} + T^{(j)}$ , where the subscript on  $h^{BR}$  denotes the number of electrons in the central field, and assume (1.6) to hold. Then

$$\begin{aligned} \inf \sigma(h_N^{BR}) &\leq \inf \sigma_{ess}(h_N^{BR}) \leq \inf \sigma(h_{N-1}^{BR} + T^{(j)}) \\ &= \inf \sigma(h_{N-1}^{BR}) + m. \end{aligned} \quad (1.8)$$

By induction (corresponding to successive removal of an electron) we get

$$\inf \sigma(h_{N-1}^{BR}) \leq \inf \sigma(h_{N-1-N'}^{BR}) + N'm, \quad 0 \leq N' < N - 1. \quad (1.9)$$

Since for a  $K$ -cluster decomposition of this specific form one has  $T + a_d = h_{N-(K-1)}^{BR} + T^{(1)} + \dots + T^{(K-1)}$ , it follows that  $\inf \sigma(T + a_d) = \inf \sigma(h_{N-(K-1)}^{BR}) + (K - 1)m \geq \inf \sigma(h_{N-1}^{BR}) + m \geq \Sigma_0$ .

Assume now cluster decompositions  $d$  with  $\#C_1 = N + 1 - (K - 1)$  fixed ( $K \in \{3, \dots, N\}$ ) but where  $\#C_i > 1$  for at least one  $i > 1$ . Then  $T + a_d$  is increased by (nonnegative) electron-electron interaction terms  $v^{(kl)}$  as compared to the  $K$ -cluster decompositions considered above, such that  $\inf \sigma(T + a_d)$  is higher (or equal) than for the case  $\#C_i = 1$ ,  $i = 2, \dots, K$ . Therefore, cluster decompositions with  $\#C_i > 1$  (for some  $i > 1$ ) do not contribute to  $\Sigma_1$ , such that, together with (1.9),  $\Sigma_1 = \Sigma_0$  is proven.

Let us embark on the proof of Theorem 1. The required lemmata will bear the same numbers as in [14].

We say that an operator  $\mathcal{O}$  is  $\frac{1}{R}$ -bounded if  $\mathcal{O}$  is bounded by  $\frac{c}{R}$  with some constant  $c > 0$ .

(a) In order to prove the 'hard part' of the HVZ theorem,  $\sigma_{ess}(h^{BR}) \subset [\Sigma_0, \infty)$ , we start by noting that the potential of  $h^{BR}$  is  $T$ -form bounded with form bound  $c < 1$  if  $\gamma < \gamma_{BR}$ . With  $\psi_+ \in \Lambda_{+,N} \mathcal{A}(H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^4)^N$ , this follows from the estimates [4, 25, 13] (using that  $V^{(k)} \leq 0$  and  $V^{(kl)} \geq 0$ ),

$$\begin{aligned} (\psi_+, \left( \sum_{k=1}^N V^{(k)} + \sum_{k>l=1}^N V^{(kl)} \right) \psi_+) &\leq \sum_{k>l=1}^N \frac{e^2}{\gamma_{BR}} (\psi_+, E_{p_1} \psi_+) \\ &= \frac{N-1}{2} \frac{e^2}{\gamma_{BR}} (\psi_+, T \psi_+) \\ (\psi_+, \left( \sum_{k=1}^N V^{(k)} + \sum_{k>l=1}^N V^{(kl)} \right) \psi_+) &\geq -\frac{\gamma}{\gamma_{BR}} \sum_{k=1}^N (\psi_+, E_{p_1} \psi_+) \\ &= -\frac{\gamma}{\gamma_{BR}} (\psi_+, T \psi_+) \end{aligned} \quad (1.10)$$

such that  $c := \max\{\frac{\gamma}{\gamma_{BR}}, \frac{N-1}{2} \frac{e^2}{\gamma_{BR}}\}$ .  $c < 1$  requires  $\gamma < \gamma_{BR}$  for all physical values of  $N$  ( $N < 250$ ). From (1.10),  $h^{BR} \geq 0$  for  $\gamma \leq \gamma_{BR}$ . In order to establish Persson's theorem (proven in [5] for Schrödinger operators and termed Lemma 2 in [14]),

$$\inf \sigma_{ess}(h^{BR}) = \lim_{R \rightarrow \infty} \inf_{\|\varphi\|=1} (\varphi, h^{BR} \varphi) \tag{1.11}$$

if  $\varphi \in \mathcal{A}(C_0^\infty(\mathbb{R}^{3N} \setminus B_R(0)) \otimes \mathbb{C}^{2N})$  where  $B_R(0) \subset \mathbb{R}^{3N}$  is a ball of radius  $R$  centered at the origin, we need the fact that the Weyl sequence  $\varphi_n$  for a  $\lambda$  in the essential spectrum of  $h^{BR}$  can be chosen such that it is supported outside a ball  $B_n(0)$ :

LEMMA 1. *Let  $h^{BR} = T + V$ , let  $V$  be relatively form bounded with respect to  $T$ . Then  $\lambda \in \sigma_{ess}(h^{BR})$  iff there exists a sequence of functions  $\varphi_n \in \mathcal{A}(C_0^\infty(\mathbb{R}^{3N} \setminus B_n(0)) \otimes \mathbb{C}^{2N})$  with  $\|\varphi_n\| = 1$  such that*

$$\|(h^{BR} - \lambda) \varphi_n\| \rightarrow 0 \quad \text{as } n \rightarrow \infty. \tag{1.12}$$

If such  $\varphi_n$  exist they form a Weyl sequence because  $\varphi_n$  converge weakly to zero [14]. For the proof of the converse direction, let  $\lambda \in \sigma_{ess}(h^{BR})$  be characterized by a Weyl sequence  $\psi_n \in \mathcal{A}(C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^2)^N$ ,  $\|\psi_n\| = 1$ , with  $\psi_n \xrightarrow{w} 0$  and  $\|(h^{BR} - \lambda)\psi_n\| \rightarrow 0$  as  $n \rightarrow \infty$ . Let  $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_N) \in \mathbb{R}^{3N}$  be the coordinates of the  $N$  electrons and define a smooth symmetric auxiliary function  $\chi_0 \in C_0^\infty(\mathbb{R}^{3N})$  mapping to  $[0, 1]$  by means of

$$\chi_0\left(\frac{\mathbf{x}}{n}\right) = \begin{cases} 1, & x \leq n \\ 0, & x > 2n \end{cases} \tag{1.13}$$

where  $x = |\mathbf{x}| = \sqrt{x_1^2 + \dots + x_N^2}$ . Then we set  $\chi_n(\mathbf{x}) := 1 - \chi_0(\mathbf{x}/n)$  and claim that a subsequence of the sequence  $\varphi_n := \psi_n \chi_n \in \mathcal{A}(C_0^\infty(\mathbb{R}^{3N} \setminus B_n(0)) \otimes \mathbb{C}^{2N})$  satisfies the requirements of Lemma 1.

In order to show that  $\|(h^{BR} - \lambda)\varphi_n\| = \|\chi_n(h^{BR} - \lambda)\psi_n + [h^{BR}, \chi_0]\psi_n\| \rightarrow 0$  for  $n \rightarrow \infty$ , we have to estimate the single-particle contributions  $\|[T^{(k)}, \chi_0]\psi_n\|$  and  $\|[b_{1m}^{(k)}, \chi_0]\psi_n\|$ . With  $b_{1m}^{(k)}$  of the form  $B_k \frac{1}{x_k} B_k$  where  $B_k \in \{A_k, G_k\}$  is a bounded multiplication operator in momentum space, we have to consider commutators of the type  $p_k[B_k, \chi_0]$  which are multiplied by bounded operators. These commutators are shown to be  $\frac{1}{n}$ -bounded in the same way as for  $N = 2$  [14], by working in momentum space and introducing the  $N$ -dimensional Fourier transform (marked by a hat) of the Schwartz function  $\chi_0$ ,

$$\widehat{\left(\chi_0\left(\frac{\cdot}{n}\right)\right)}(\mathbf{p}) = \frac{1}{(2\pi)^{3N/2}} \int_{\mathbb{R}^{3N}} d\mathbf{x} e^{-i\mathbf{p}\mathbf{x}} \chi_0\left(\frac{\mathbf{x}}{n}\right) = n^{3N} \hat{\chi}_0(\mathbf{p}_1 n, \dots, \mathbf{p}_N n), \tag{1.14}$$

where  $\mathbf{p} = (\mathbf{p}_1, \dots, \mathbf{p}_N)$ , and by using the mean value theorem to estimate the difference  $|B_k(\mathbf{p}_k) - B_k(\mathbf{p}_{k'})|$  respective  $|T^{(k)}(\mathbf{p}_k) - T^{(k)}(\mathbf{p}_{k'})|$ . The two-particle contributions  $\|[v^{(kl)}, \chi_0]\psi_n\|$  can, according to the representation (1.3)

of  $v^{(kl)}$ , also be split into single-particle commutators  $p_k[B_k, \chi_0]$  multiplied by bounded operators. Their estimate as well as the remaining parts of the proof of Lemma 1 for  $N > 2$  (in particular the normalizability of  $\varphi_n$  for sufficiently large  $n$  which relies on the relative form boundedness of the total potential) can be mimicked from the case of  $N = 2$ .

Our aim is a generalization of the localization formula of Lewis et al [16] to the operator  $h^{BR}$ . We introduce the Ruelle-Simon [22] partition of unity  $(\phi_j)_{j=0, \dots, N} \in C^\infty(\mathbb{R}^{3N})$  which is subordinate to the two-cluster decompositions (1.4). It is defined on the unit sphere in  $\mathbb{R}^{3N}$  and has the following properties (see e.g. [5, p.33], [24])

$$\sum_{j=0}^N \phi_j^2 = 1, \quad \phi_j(\lambda \mathbf{x}) = \phi_j(\mathbf{x}) \quad \text{for } x = 1 \text{ and } \lambda \geq 1,$$

$$\text{supp } \phi_j \cap \mathbb{R}^{3N} \setminus B_1(0) \subseteq \{\mathbf{x} \in \mathbb{R}^{3N} \setminus B_1(0) : |\mathbf{x}_k - \mathbf{x}_l| \geq Cx \text{ for all } k \in C_{1j} \quad (1.15)$$

$$\text{and } l \in C_{2j}, \text{ and } x_k \geq Cx \text{ for all } k \in C_{2j}\}, \quad j = 0, 1, \dots, N$$

where  $C$  is a constant and it is again assumed that the nucleus belongs to cluster  $C_{1j}$ . Then we have

LEMMA 3. *Let  $h^{BR} = T + a_j + r_j$ ,  $(\phi_j)_{j=0, \dots, N}$  be the Ruelle-Simon partition of unity and  $\varphi \in \mathcal{A}(C_0^\infty(\mathbb{R}^{3N} \setminus B_R(0)) \otimes \mathbb{C}^{2N})$  with  $R > 1$ . Then, with some constant  $c$ ,*

$$|(\phi_j \varphi, r_j \phi_j \varphi)| \leq \frac{c}{R} \|\varphi\|^2, \quad j = 0, \dots, N. \quad (1.16)$$

There are two possibilities.  $r_j$  may (a) consist of terms  $b_{1m}^{(k)}$  for some  $k \in C_{2j}$ , or (b) of terms  $v^{(kl)}$  with particles  $k$  and  $l$  in different clusters. For the proof, all summands of  $r_j$  are estimated separately. For each summand of  $r_j$  (to a given cluster decomposition  $j$ ), a specific smooth auxiliary function  $\chi$  mapping to  $[0, 1]$  is introduced which is unity on the support of  $\phi_j \varphi$ , such that  $\phi_j \varphi \chi = \phi_j \varphi$ . In case (a) we have  $\text{supp } \phi_j \varphi \subset \mathbb{R}^{3N} \setminus B_R(0) \cap \{x_k \geq Cx\}$ , i.e.  $x_k \geq CR$ . Therefore we define the (single-particle) function

$$\chi_k\left(\frac{\mathbf{x}_k}{R}\right) := \begin{cases} 0, & x_k < CR/2 \\ 1, & x_k \geq CR \end{cases} \quad (1.17)$$

With  $b_{1m}^{(k)}$  of the form  $B_k \frac{1}{x_k} B_k$  we have to consider

$$(\phi_j \varphi, B_k \frac{1}{x_k} B_k \chi_k \phi_j \varphi) = (\phi_j \varphi, B_k \frac{1}{x_k} \chi_k B_k \phi_j \varphi) + (\phi_j \varphi, B_k \frac{1}{x_k} [B_k, 1 - \chi_k] \phi_j \varphi).$$

The first term is uniformly  $2/R$ -bounded by the choice (1.17) of  $\chi_k$ , whereas the second term can be estimated in momentum space as in the two-electron case (respective in the proof of Lemma 1).

In case (b) we have  $\text{supp } \phi_j \varphi \subset \mathbb{R}^{3N} \setminus B_R(0) \cap \{|\mathbf{x}_k - \mathbf{x}_l| \geq Cx\}$ , i.e.  $|\mathbf{x}_k - \mathbf{x}_l| \geq CR$ . Accordingly, we take

$$\chi_{kl}\left(\frac{\mathbf{x}_k - \mathbf{x}_l}{R}\right) := \begin{cases} 0, & |\mathbf{x}_k - \mathbf{x}_l| < CR/2 \\ 1, & |\mathbf{x}_k - \mathbf{x}_l| \geq CR \end{cases} \quad (1.18)$$

With the representation (1.3) of  $v^{(kl)}$ , we have to estimate commutators of the type  $p_k[B_k B_l, 1 - \chi_{kl}]$ . The proof of their uniform  $1/R$ -boundedness can be copied from the two-electron case.

The second ingredient of the localization formula is an estimate for the commutator of  $\phi_j$  with  $h^{BR}$ :

LEMMA 4. *Let  $h^{BR}$  from (1.2) and  $(\phi_j)_{j=0,\dots,N}$  be the Ruelle-Simon partition of unity. Then for  $\varphi \in \mathcal{A}(C_0^\infty(\mathbb{R}^{3N} \setminus B_R(0)) \otimes \mathbb{C}^{2N})$  and  $R > 2$  one has*

$$\begin{aligned}
 (a) \quad & \left| \sum_{j=0}^N (\phi_j \varphi, [T, \phi_j] \varphi) \right| \leq \frac{c}{R^2} \|\varphi\|^2 \\
 (b) \quad & |(\phi_j \varphi, [b_{1m}^{(k)}, \phi_j] \varphi)| \leq \frac{c}{R} \|\varphi\|^2 \\
 (c) \quad & |(\phi_j \varphi, [v^{(kl)}, \phi_j] \varphi)| \leq \frac{c}{R} \|\varphi\|^2
 \end{aligned} \tag{1.19}$$

where  $c$  is a generic constant.

Item (a) is proven in [16]. For items (b) and (c) we define the smooth auxiliary  $N$ -particle function  $\chi$  mapping to  $[0, 1]$ ,

$$\chi\left(\frac{\mathbf{x}}{R}\right) := \begin{cases} 0, & x < R/2 \\ 1, & x \geq R \end{cases} . \tag{1.20}$$

Then  $\phi_j \varphi = \phi_j \varphi \chi$  on  $\text{supp } \varphi$ , and therefore  $(\phi_j \varphi, [b_{1m}^{(k)}, \phi_j] \varphi) = (\phi_j \varphi, [b_{1m}^{(k)}, \phi_j \chi] \varphi)$ . The  $\frac{1}{R}$ -estimate, claimed in (1.19), relies on the scaling property  $\phi_j(\mathbf{x})\chi(\frac{\mathbf{x}}{R}) = \phi_j(\frac{\mathbf{x}}{R/2})\chi(\frac{\mathbf{x}}{R})$  which holds for  $R > 2$  since  $\text{supp } \chi$  (and hence  $\text{supp } \phi_j \chi$ ) is outside  $B_{R/2}(0)$ . Thus, working in coordinate space and using the mean value theorem, we get the estimate

$$|(\phi_j \chi)(\mathbf{x}_1, \dots, \mathbf{x}_k, \dots, \mathbf{x}_N) - (\phi_j \chi)(\mathbf{x}_1, \dots, \mathbf{x}'_k, \dots, \mathbf{x}_N)| \leq |\mathbf{x}_k - \mathbf{x}'_k| \frac{c_0}{R} \tag{1.21}$$

(only the  $k$ -th coordinate in the second entry of the l.h.s. is primed). Since (1.21) holds for arbitrary  $k \in \{1, \dots, N\}$ , the proof of (b) and (c) can be carried out in the same way as done in the two-electron case, by estimating the kernel of  $B_k \in \{A_k, G_k\}$  in coordinate space by  $c/|\mathbf{x}_k - \mathbf{x}'_k|^3$  (using asymptotic analysis [19]) and subsequently proving the uniform  $\frac{1}{R}$ -boundedness of  $[B_k, \phi_j \chi] \frac{1}{x_k}$  respective  $[B_k, \phi_j \chi] \frac{1}{|\mathbf{x}_k - \mathbf{x}_l|}$ .

With Lemmata 3 and 4 we obtain the desired localization formula for  $h^{BR}$ ,

$$\begin{aligned}
 (\varphi, h^{BR} \varphi) &= \sum_{j=0}^N (\phi_j \varphi, (T + a_j) \phi_j \varphi) \\
 &+ \sum_{j=0}^N (\phi_j \varphi, r_j \phi_j \varphi) - \sum_{j=0}^N (\phi_j \varphi, [h^{BR}, \phi_j] \varphi)
 \end{aligned} \tag{1.22}$$

$$= \sum_{j=0}^N (\phi_j \varphi, (T + a_j) \phi_j \varphi) + O\left(\frac{1}{R}\right) \|\varphi\|^2$$

for  $R > 2$ . From Persson's theorem (1.11) and the definition (1.5) of  $\Sigma_0$  we therefore get

$$\begin{aligned} \inf \sigma_{ess}(h^{BR}) &= \lim_{R \rightarrow \infty} \inf_{\|\varphi\|=1} \sum_{j=0}^N (\phi_j \varphi, (T + a_j) \phi_j \varphi) \\ &\geq \Sigma_0 \sum_{j=0}^N (\phi_j \varphi, \phi_j \varphi) = \Sigma_0 \end{aligned} \quad (1.23)$$

which proves the inclusion  $\sigma_{ess}(h^{BR}) \subset [\Sigma_0, \infty)$ .

(b) We now turn to the 'easy part' of the proof where we have to verify  $[\Sigma_0, \infty) \subset \sigma_{ess}(h^{BR})$ .

We start by showing that for every  $j \in \{0, 1, \dots, N\}$ ,  $\sigma(T + a_j)$  is continuous, i.e. for any  $\lambda \in [\inf \sigma(T + a_j), \infty)$  one has  $\lambda \in \sigma(T + a_j)$ . If the cluster  $C_{2j}$  consists of a single electron  $j$ , then  $T + a_j = T^{(j)} + h_{N-1}^{BR}$  where  $h_{N-1}^{BR}$  does not contain any interaction with electron  $j$ . The continuity of  $\sigma(T^{(j)} + h_{N-1}^{BR})$  then follows from the continuity of  $\sigma(T^{(j)})$  in the same way as for  $N = 2$ .

In the case  $j = 0$  where  $C_{2j}$  contains  $N$  electrons, the total momentum  $\mathbf{p}_0$  of  $C_{2j}$  is well-defined and commutes with its Hamiltonian  $h_0 := T + \sum_{k>l=1}^N v^{(kl)} = T + a_0$ . This follows from the absence of any central potential in  $h_0$  and from the symmetry of  $v^{(kl)}$ ,

$$\left[ (-i\nabla_{\mathbf{x}_k} - i\nabla_{\mathbf{x}_l}), \frac{1}{|\mathbf{x}_k - \mathbf{x}_l|} \right] \psi(\mathbf{x}) = (-i\nabla_{\mathbf{x}_k} - i\nabla_{\mathbf{x}_l}) \left( \frac{1}{|\mathbf{x}_k - \mathbf{x}_l|} \right) \psi(\mathbf{x}) = 0 \cdot \psi(\mathbf{x}) = 0. \quad (1.24)$$

Thus the eigenfunctions to  $h_0$  can be chosen as eigenfunctions of  $\mathbf{p}_0$ . For  $p_0 \geq 0$  the associated center of mass energy of  $C_{2j}$  is continuous. Therefore,  $\inf \sigma(h_0)$  is attained for  $p_0 = 0$  and  $\sigma(h_0)$  is continuous.

Let  $\lambda \in [\Sigma_0, \infty)$ . We have  $\Sigma_0 = \inf \sigma(T + a_j)$  for a specific  $j \in \{0, \dots, N\}$ . Then  $\lambda \in \sigma(T + a_j)$ , i.e. there exists a defining sequence  $\varphi_n(\mathbf{x}) \in C_0^\infty(\mathbb{R}^{3N}) \otimes \mathbb{C}^{2N}$  with  $\|\varphi_n\| = 1$  and  $\|(T + a_j - \lambda) \varphi_n\| \rightarrow 0$  for  $n \rightarrow \infty$ .

Assume that  $l$  electrons belong to cluster  $C_{2j}$  which we will enumerate by  $N - l + 1, \dots, N$ , and follow [10] to define the unitary translation operator  $T_{\mathbf{a}}$  by means of

$$T_{\mathbf{a}} \psi(\mathbf{x}_1, \dots, \mathbf{x}_N) = \psi(\mathbf{x}_1, \dots, \mathbf{x}_{N-l}, \mathbf{x}_{N-l+1} - \mathbf{a}, \dots, \mathbf{x}_N - \mathbf{a}) \quad (1.25)$$

with  $|\mathbf{a}| = a$  and let  $\mathbf{a}_l := (\mathbf{a}, \dots, \mathbf{a}) \in \mathbb{R}^{3l}$ . Hence cluster  $C_{2j}$  moves to infinity as  $a \rightarrow \infty$ .

Let  $\psi_n^{(a)} := T_{\mathbf{a}}\varphi_n$  and  $\mathcal{A}\psi_n^{(a)}$  be the antisymmetric function constructed from  $\psi_n^{(a)}$ . We claim that  $\mathcal{A}\psi_n^{(a)}$  is a defining sequence for  $\lambda \in \sigma(h^{BR})$ . It is sufficient (as shown below) to prove that  $\psi_n^{(a)}$  has this property. We have trivially  $\|\psi_n^{(a)}\| = \|\varphi_n\|$  and we have to show that  $\|(h^{BR} - \lambda)\psi_n^{(a)}\| \rightarrow 0$  for  $n \rightarrow \infty$  and a suitably large  $a$ . We have

$$\|(h^{BR} - \lambda)\psi_n^{(a)}\| \leq \|(T + a_j - \lambda)\psi_n^{(a)}\| + \|r_j\psi_n^{(a)}\|. \tag{1.26}$$

$T$  commutes with  $T_{\mathbf{a}}$  because  $T$  is a multiplication operator in momentum space. Since the central potentials contained in  $a_j$  are not affected by  $T_{\mathbf{a}}$  (because  $T_{\mathbf{a}}$  does not act on the particle coordinates of cluster  $C_{1j}$ ), we also have  $[T_{\mathbf{a}}, a_j] = 0$ . In fact, assuming e.g. that electrons  $k$  and  $l$  are in cluster  $C_{2j}$  and using the representation (1.3) for  $v^{(kl)}$  we have with  $T_{\mathbf{a}}^*T_{\mathbf{a}} = 1$  and  $B_k, \tilde{B}_k \in \{A_k, G_k\}$ ,

$$\begin{aligned} T_{\mathbf{a}}^*B_k\tilde{B}_l \frac{1}{|\mathbf{x}_k - \mathbf{x}_l|} B_k\tilde{B}_l T_{\mathbf{a}} &= B_k\tilde{B}_l T_{\mathbf{a}}^* \frac{1}{|\mathbf{x}_k - \mathbf{x}_l|} T_{\mathbf{a}} B_k\tilde{B}_l \\ &= B_k\tilde{B}_l \frac{1}{|\mathbf{x}_k + \mathbf{a} - (\mathbf{x}_l + \mathbf{a})|} B_k\tilde{B}_l = B_k\tilde{B}_l \frac{1}{|\mathbf{x}_k - \mathbf{x}_l|} B_k\tilde{B}_l \end{aligned} \tag{1.27}$$

such that  $[T_{\mathbf{a}}, v^{(kl)}] = 0$ . Then, given some  $\epsilon > 0$ , the first term of (1.26) reduces to

$$\|(T + a_j - \lambda)T_{\mathbf{a}}\varphi_n\| = \|T_{\mathbf{a}}(T + a_j - \lambda)\varphi_n\| \leq \|T_{\mathbf{a}}\| \|(T + a_j - \lambda)\varphi_n\| < \epsilon/2 \tag{1.28}$$

if  $n > N_0$  for  $N_0$  sufficiently large.

For the second term in (1.26) we note that  $r_j$  consists of terms  $b_{1m}^{(k)}$  with  $k \notin C_{1j}$  and terms  $v^{(kk')}$  with  $k \in C_i, k' \in C_{i'}, i \neq i'$ . Moreover, since  $a_j$  does not contain any intercluster interactions, we can choose  $\varphi_n = \varphi_1^{(n)} \cdot \varphi_2^{(n)}$  as a product of functions ( $\varphi_1^{(n)} \in C_0^\infty(\mathbb{R}^{3(N-l)} \otimes \mathbb{C}^{2(N-l)})$ ,  $\varphi_2^{(n)} \in C_0^\infty(\mathbb{R}^{3l} \otimes \mathbb{C}^{2l})$ ) each of which describing the electrons in cluster  $C_{1j}$  respective  $C_{2j}$ . Let  $\text{supp } \varphi_i^{(n)} \subset B_{R_i}(0)$  for a suitable  $R_i$ .

Consider  $\|b_{1m}^{(k)}\psi_n^{(a)}\|$  with  $k \in C_{2j}$ . We have  $\text{supp } T_{\mathbf{a}}\varphi_2^{(n)} \subset B_{R_2}(\mathbf{a}_l)$ . Let  $a > 2R_2$ . For all  $k' \in C_{2j}$ , on the support of  $T_{\mathbf{a}}\varphi_2^{(n)}$  we have  $R_2 > |\mathbf{x}_{k'} - \mathbf{a}| \geq a - x_{k'}$  and thus  $x_{k'} > a - R_2$ . Therefore we can write  $\text{supp } T_{\mathbf{a}}\varphi_2^{(n)} \subset \mathbb{R}^{3l} \setminus B_{|\mathbf{a}_l| - R_2}(0) \cap \{x_{k'} > a - R_2 \ \forall k' \in C_{2j}\}$ . Assume we can prove

LEMMA 5. *Let  $\varphi \in C_0^\infty(\Omega) \otimes \mathbb{C}^{2l}$  with  $\Omega := \{\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_l) \in \mathbb{R}^{3l} : x_i > R \ \forall i = 1, \dots, l\}$  and  $R > 1$ . Then for  $k \in \{1, \dots, l\}$  and some constant  $c$ ,*

$$\|b_{1m}^{(k)}\varphi\| \leq \frac{c}{R}\|\varphi\|. \tag{1.29}$$

Since  $b_{1m}^{(k)}$  acts only on  $T_{\mathbf{a}}\varphi_2^{(n)}$  we obtain

$$\|b_{1m}^{(k)}T_{\mathbf{a}}\varphi_n\| = \|\varphi_1^{(n)}\| \|b_{1m}^{(k)}T_{\mathbf{a}}\varphi_2^{(n)}\| \leq \frac{c}{a - R_2} \|T_{\mathbf{a}}\varphi_2^{(n)}\| < \frac{2c}{a} \tag{1.30}$$

because the  $\varphi_i^{(n)}$  are normalized. As a consequence, for any  $k \in C_{2j}$ , the l.h.s. of (1.30) can be made smaller than  $\epsilon/4l$  for sufficiently large  $a$ .

For the proof of Lemma 5 or, equivalently, of  $|(\phi, b_{1m}^{(k)}\varphi)| \leq \frac{\epsilon}{R} \|\varphi\| \|\phi\|$  for all  $\phi \in (C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^2)^l$ , we note that the basic difference to the respective assertion for  $N = 2$  lies in the possible multiparticle nature of  $\phi$  and  $\varphi$ . However, the property of the domain  $\Omega$  of  $\varphi$  allows for the introduction of the (single-particle) smooth auxiliary function (mapping to  $[0, 1]$ ),

$$\chi\left(\frac{\mathbf{x}_k}{R}\right) := \begin{cases} 0, & x_k < R/2 \\ 1, & x_k \geq R \end{cases}, \tag{1.31}$$

such that  $\varphi\chi = \varphi$ . Then the proof can be copied from the two-electron case. For the two-particle interaction contained in  $r_j$ , one has

LEMMA 6. *Let  $\psi_n^{(a)} = T_{\mathbf{a}}\varphi_n = T_{\mathbf{a}}\varphi_1^{(n)}\varphi_2^{(n)}$  as defined above. Then for all  $\varphi \in (C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^2)^N$  and  $a > 4R$ ,*

$$|(\varphi, v^{(kk')}\psi_n^{(a)})| \leq \frac{c_0}{a - 2R} \|\varphi\| \|\psi_n^{(a)}\| \tag{1.32}$$

with some positive constants  $c_0$  and  $R$ , provided particles  $k$  and  $k'$  belong to two different clusters.

For the proof of Lemma 6, we need again a suitable auxiliary function  $\chi$ . Let  $k' \in C_{1j}$ ,  $k \in C_{2j}$ . We have  $\text{supp } \varphi_1^{(n)}\varphi_2^{(n)} \subset B_{R_1}(0) \times B_{R_2}(0)$  and  $\text{supp } T_{\mathbf{a}}\varphi_1^{(n)}\varphi_2^{(n)} \subset B_{R_1}(0) \times B_{R_2}(\mathbf{a}_l)$ . Hence  $x_{k'} < R_1$  and  $x_k > a - R_2$ . So the inter-electron separation can be estimated by  $|\mathbf{x}_k - \mathbf{x}_{k'}| \geq x_k - x_{k'} > a - R_2 - R_1$ . Let  $R := \max\{R_1, R_2\}$  and  $\tilde{a} := a - 2R$ . Define

$$\chi_{kk'}\left(\frac{\mathbf{x}_k - \mathbf{x}_{k'}}{\tilde{a}}\right) := \begin{cases} 0, & |\mathbf{x}_k - \mathbf{x}_{k'}| < \tilde{a}/2 \\ 1, & |\mathbf{x}_k - \mathbf{x}_{k'}| \geq \tilde{a} \end{cases}. \tag{1.33}$$

Then  $\chi_{kk'}$  is unity on the support of  $\psi_n^{(a)}$ , such that  $\chi_{kk'}\psi_n^{(a)} = \psi_n^{(a)}$ . With this function, the proof of Lemma 6 is done exactly as in the two-electron case. Collecting results, we obtain for  $n > N_0$  and  $a > 4R$  sufficiently large

$$\begin{aligned} \|(h^{BR} - \lambda)\psi_n^{(a)}\| &\leq \|(T + a_j - \lambda)\varphi_n\| + l \frac{2c}{a} \\ &+ \tilde{N} \frac{2c_0}{a} \|\psi_n^{(a)}\| < \epsilon \end{aligned} \tag{1.34}$$

where  $\tilde{N}$  is the total number of two-electron intercluster interactions. This proves that  $\lambda \in \sigma(h^{BR})$ . Since  $\lambda \in [\Sigma_0, \infty)$  was chosen arbitrarily, we therefore have  $[\Sigma_0, \infty) \subset \sigma(h^{BR})$ , indicating that  $\sigma(h^{BR})$  has to be continuous in  $[\Sigma_0, \infty)$ . Consequently,  $[\Sigma_0, \infty) \subset \sigma_{ess}(h^{BR})$  which completes the proof of Theorem 1.

We are left to show that the defining sequence for  $\lambda$  can be chosen to be antisymmetric. We write  $\mathcal{A}\psi_n^{(a)} = c_1 \sum_{\sigma \in \mathcal{P}} \text{sign}(\sigma) \psi_{n,\sigma}^{(a)}$  where  $\psi_{n,\sigma}^{(a)} = \psi_n^{(a)}(\mathbf{x}_{\sigma(1)}, \dots, \mathbf{x}_{\sigma(N)})$  with  $\mathcal{P}$  the permutation group of the numbers  $1, \dots, N$ , and  $c_1$  is a normalization constant. Since  $h^{BR}$  is symmetric upon particle exchange we have

$$\|(h^{BR} - \lambda) \mathcal{A}\psi_n^{(a)}\| \leq c_1 \sum_{\sigma \in \mathcal{P}} \|(h^{BR} - \lambda) \psi_{n,\sigma}^{(a)}\| = c_1 (\#\sigma) \|(h^{BR} - \lambda) \psi_n^{(a)}\|. \tag{1.35}$$

By (1.34) this can be made smaller than  $\epsilon$  since the number  $\#\sigma$  of permutations is finite.

It remains to prove that  $\mathcal{A}\psi_n^{(a)}$  is normalizable. Without restriction we can assume in the factorization  $\varphi_n = \varphi_n^{(1)} \cdot \varphi_n^{(2)}$  that  $\varphi_n^{(1)}$  and  $\varphi_n^{(2)}$  are antisymmetric, such that  $\sigma$  can be restricted to the permutation of coordinates relating to different clusters. We claim that scalar products of the form

$$\begin{aligned} &(\varphi_1^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_{N-l}) \varphi_2^{(n)}(\mathbf{x}_{N-l+1} - \mathbf{a}, \dots, \mathbf{x}_N - \mathbf{a}), \varphi_1^{(n)}(\mathbf{x}_{\sigma(1)}, \dots, \mathbf{x}_{\sigma(N-l)}) \\ &\quad \cdot \varphi_2^{(n)}(\mathbf{x}_{\sigma(N-l+1)} - \mathbf{a}, \dots, \mathbf{x}_{\sigma(N)} - \mathbf{a})) \end{aligned} \tag{1.36}$$

where  $\exists k \in \{1, \dots, N-l\}$  and  $k' \in \{N-l+1, \dots, N\}$  such that  $\sigma(k) \in \{N-l+1, \dots, N\}$  and  $\sigma(k') \in \{1, \dots, N-l\}$ , can be made arbitrarily small for a suitably large  $a$ . In fact, since  $x_{\sigma(k')} < R_1$  on  $\text{supp } \varphi_1^{(n)}$  and  $|\mathbf{x}_{\sigma(k')} - \mathbf{a}| < R_2$  on  $\text{supp } \varphi_2^{(n)}$ , we have  $\int_{\mathbb{R}^3} d\mathbf{x}_{\sigma(k')} \overline{\varphi_1^{(n)}}(\dots, \mathbf{x}_{\sigma(k')}, \dots) \varphi_2^{(n)}(\dots, \mathbf{x}_{\sigma(k')} - \mathbf{a}, \dots) = 0$  if  $a > R_1 + R_2$ . Thus we get

$$\|\mathcal{A}\psi_n^{(a)}\|^2 = c_1^2 \sum_{\sigma \in \mathcal{P}} (\psi_{n,\sigma}^{(a)}, \psi_{n,\sigma}^{(a)}) \tag{1.37}$$

since all cross terms vanish for sufficiently large  $a$ . This guarantees the normalizability of  $\mathcal{A}\psi_n^{(a)}$ .

## 2 THE TWO-ELECTRON JANSEN-HESS OPERATOR

The Jansen-Hess operator includes the terms which are quadratic in the fine structure constant  $e^2$ . We restrict ourselves in this section to the two-electron ion and write the Jansen-Hess operator  $H^{(2)}$  in the following form [11]

$$H^{(2)} = H_2^{BR} + \Lambda_{+,2} \left( \sum_{k=1}^2 B_{2m}^{(k)} + C^{(12)} \right) \Lambda_{+,2} \tag{2.1}$$

$$B_{2m}^{(k)} := \frac{\gamma^2}{8\pi^2} \left\{ \frac{1}{x_k} \left( 1 - \frac{\boldsymbol{\alpha}^{(k)} \mathbf{p}_k + \beta^{(k)} m}{E_{p_k}} \right) V_{10,m}^{(k)} + V_{10,m}^{(k)} \left( 1 - \frac{\boldsymbol{\alpha}^{(k)} \mathbf{p}_k + \beta^{(k)} m}{E_{p_k}} \right) \frac{1}{x_k} \right\}$$

$$V_{10,m}^{(k)} := 2\pi^2 \int_0^\infty dt e^{-tE_{p_k}} \frac{1}{x_k} e^{-tE_{p_k}}$$

where  $H_2^{BR}$  is the Brown-Ravenhall operator from (1.1) indexed by 2 (for  $N = 2$ ),  $\Lambda_{+,2} = \Lambda_+^{(1)}\Lambda_+^{(2)}$  and  $V_{10,m}^{(k)}$  is a bounded single-particle integral operator. The two-particle second-order contribution  $C^{(12)}$  is given by

$$C^{(12)} := \sum_{k=1}^2 (V^{(12)} \Lambda_-^{(k)} F_0^{(k)} + F_0^{(k)} \Lambda_-^{(k)} V^{(12)}) \quad (2.2)$$

$$F_0^{(k)} := -\frac{1}{2\pi} \int_{-\infty}^\infty d\eta \frac{1}{D_0^{(k)} + i\eta} V^{(k)} \frac{1}{D_0^{(k)} + i\eta}$$

and  $\Lambda_-^{(k)} = 1 - \Lambda_+^{(k)}$ . Also  $F_0^{(k)}$  is a bounded single-particle integral operator. In the same way as for the Brown-Ravenhall operator, an equivalent operator  $h^{(2)}$  acting on the reduced spinor space  $\mathcal{A}(L_2(\mathbb{R}^3) \otimes \mathbb{C}^2)^2$ , can be defined,

$$h^{(2)} = h_2^{BR} + \sum_{k=1}^2 b_{2m}^{(k)} + c^{(12)} \quad (2.3)$$

with

$$b_{2m}^{(k)} = \frac{\gamma^2}{8\pi^2} \left\{ A_k \frac{1}{x_k} V_{10,m}^{(k)} A_k - G_k \frac{1}{x_k} \frac{\boldsymbol{\sigma}^{(k)} \mathbf{p}_k}{E_{p_k}} V_{10,m}^{(k)} A_k - A_k \frac{1}{x_k} \frac{m}{E_{p_k}} V_{10,m}^{(k)} A_k \right. \\ \left. + G_k \frac{1}{x_k} V_{10,m}^{(k)} G_k - A_k \frac{1}{x_k} \frac{\boldsymbol{\sigma}^{(k)} \mathbf{p}_k}{E_{p_k}} V_{10,m}^{(k)} G_k + G_k \frac{1}{x_k} \frac{m}{E_{p_k}} V_{10,m}^{(k)} G_k + \text{h.c.} \right\} \quad (2.4)$$

where  $A_k, G_k$  are defined below (1.2) and h.c. means Hermitean conjugate (such that  $b_{2m}^{(k)}$  is a symmetric operator). Note that, due to the presence of the projector  $\Lambda_+^{(k)}$  in (2.1),  $b_{2m}^{(k)}$  contains only even powers in  $\boldsymbol{\sigma}^{(k)}$ . In a similar way,  $c^{(12)}$  is derived from  $C^{(12)}$ . The particle mass  $m$  is assumed to be nonzero throughout (for  $m = 0$ , the spectrum of the single-particle Jansen-Hess operator is absolutely continuous with infimum zero [11]).

For potential strength  $\gamma < 0.89$  (slightly smaller than  $\gamma_{BR}$ ), it was shown [13] that the total potential of  $H^{(2)}$  (and hence also of  $h^{(2)}$ ) is relatively form bounded (with form bound smaller than 1) with respect to the kinetic energy operator. Therefore,  $h^{(2)}$  is well-defined in the form sense and is a self-adjoint operator by means of the Friedrichs extension of the restriction of  $h^{(2)}$  to  $\mathcal{A}(C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^2)^2$ . The above form boundedness guarantees the existence of a  $\mu > 0$  such that  $h^{(2)} + \mu > 0$  for  $\gamma < 0.89$ . If  $\gamma < 0.825$ , one can even choose  $\mu = 0$  [13].

Let us introduce the operator  $\tilde{h}^{(2)}$  by means of  $h^{(2)} =: \tilde{h}^{(2)} + c^{(12)}$  and define in analogy to (1.4) the two-cluster decompositions of  $\tilde{h}^{(2)}$  for  $j=0,1,2$ ,

$$\tilde{h}^{(2)} = T + a_j + r_j \quad (2.5)$$

as well as

$$\Sigma_0 := \min_j \inf \sigma(T + a_j). \tag{2.6}$$

The aim of this section is to prove

**THEOREM 2 (HVZ THEOREM FOR THE TWO-ELECTRON JANSEN-HESS OPERATOR).**

Let  $h^{(2)} = \sum_{k=1}^2 (T^{(k)} + b_{1m}^{(k)} + b_{2m}^{(k)}) + v^{(12)} + c^{(12)} = \tilde{h}^{(2)} + c^{(12)}$  be the two-electron Jansen-Hess operator with potential strength  $\gamma < 0.66$  ( $Z \leq 90$ ). Let (2.5) be the two-cluster decompositions of  $\tilde{h}^{(2)}$  and  $\Sigma_0$  from (2.6). Then the essential spectrum of  $h^{(2)}$  is given by

$$\sigma_{ess}(h^{(2)}) = [\Sigma_0, \infty). \tag{2.7}$$

We start by noting that the two-particle second-order potential  $c^{(12)}$  does not change the essential spectrum of  $h^{(2)}$  :

**PROPOSITION 1.** Let  $h^{(2)} = \tilde{h}^{(2)} + c^{(12)}$  be the two-electron Jansen-Hess operator with potential strength  $\gamma < 0.66$ . Then one has

$$\sigma_{ess}(h^{(2)}) = \sigma_{ess}(\tilde{h}^{(2)}). \tag{2.8}$$

*Proof.*

The proof is performed for the equivalent operator  $H^{(2)} =: \tilde{H}^{(2)} + \Lambda_{+,2} C^{(12)} \Lambda_{+,2}$ .

The resolvent difference

$$R_\mu := (H^{(2)} + \mu)^{-1} - (\tilde{H}^{(2)} + \mu)^{-1} \tag{2.9}$$

is bounded for  $\mu \geq 0$  since  $H^{(2)}$  as well as  $\tilde{H}^{(2)}$  are positive for  $\gamma < 0.825$  which exceeds the critical  $\gamma$  of Proposition 1. We will show that  $R_\mu$  is compact. Then, following the argumentation of [7], one can use Lemma 3 of [20, p.111] together with the strong spectral mapping theorem ([20, p.109]) to prove that the essential spectra of  $H^{(2)}$  and  $\tilde{H}^{(2)}$  coincide.

Let  $T_0 := \Lambda_{+,2} \sum_{k=1}^2 D_0^{(k)} \Lambda_{+,2}$  which is a positive operator (for  $m \neq 0$ ) on the positive spectral subspace  $\Lambda_{+,2} \mathcal{A}(H_1(\mathbb{R}^3) \otimes \mathbb{C}^4)^2$ . (The negative spectral subspace is disregarded throughout because  $H^{(2)} = 0$  on that subspace.) With the help of the second resolvent identity, one decomposes  $R_\mu$  into

$$\begin{aligned} R_\mu &= -(\tilde{H}^{(2)} + \mu)^{-1} \Lambda_{+,2} C^{(12)} \Lambda_{+,2} (H^{(2)} + \mu)^{-1} \\ &= - \left[ (\tilde{H}^{(2)} + \mu)^{-1} (T_0 + \mu) \right] \cdot \left\{ (T_0 + \mu)^{-1} \Lambda_{+,2} C^{(12)} \Lambda_{+,2} (T_0 + \mu)^{-1} \right\} \\ &\quad \cdot \left[ (T_0 + \mu) (H^{(2)} + \mu)^{-1} \right]. \end{aligned} \tag{2.10}$$

One can show (see [11, proof b] of Theorem II.1 with  $T$  replaced by  $T_0$ ) that for  $\gamma < 0.66$ , the two operators in square brackets are bounded. This relies on the relative boundedness of the total potential of  $H^{(2)}$  (respective  $\tilde{H}^{(2)}$ ) with respect to  $T_0$ , with (operator) bound less than one for  $m = 0$  ([11]; Appendix B). Due to scaling (for  $\mu = 0$ ), the boundedness of the operators in square brackets holds for all  $m$ . The operator in curly brackets is shown to be compact. To this aim it is written as

$$(T_0 + \mu)^{-1} \Lambda_{+,2} C^{(12)} \Lambda_{+,2} (T_0 + \mu)^{-1} \tag{2.11}$$

$$= (T_0 + \mu)^{-1} (T + \mu) \Lambda_{+,2} W_2 \Lambda_{+,2} (T + \mu) (T_0 + \mu)^{-1}$$

with  $W_2 := (T + \mu)^{-1} C^{(12)} (T + \mu)^{-1}$ . According to Herbst [8],  $W_2$  is decomposed into  $W_{2n} + R_n$  where  $(W_{2n})_{n \in \mathbb{N}}$  is a sequence of Hilbert-Schmidt operators satisfying  $\|W_{2n} - W_2\| \rightarrow 0$  for  $n \rightarrow \infty$ . It follows that  $W_{2n}$  is compact such that also  $W_2$  is compact (see e.g. [15, III.4.2, V.2.4]).  $W_{2n}$  is defined by regularizing the Coulomb potential by means of  $\frac{1}{x} e^{-\epsilon x}$  and by introducing convergence generating functions  $e^{-\epsilon p}$  in momentum space, where  $\epsilon := \frac{1}{n} > 0$  is a small quantity. Details of the proof are found in [11]. The adjacent factors of  $W_2$  in (2.11) are easily seen to be bounded for  $\mu = 0$ . Since  $\Lambda_{+,2} = \Lambda_{+,2}^2$  commutes with  $T$ , one has e.g.  $\Lambda_{+,2} T T_0^{-1} = (\Lambda_{+,2} T \Lambda_{+,2}) T_0^{-1} = T_0 T_0^{-1} = 1$ . Therefore, the operator in curly brackets and hence  $R_\mu$  is proven to be compact for  $\mu = 0$ .  $\square$

*Proof of Theorem 2.* With Proposition 1 at hand, it remains to prove the HVZ theorem for the operator  $\tilde{h}^{(2)}$ , which in fact holds for all  $\gamma < \gamma_{BR}$ .

We proceed along the same lines as done in the proof of the HVZ theorem for the Brown-Ravenhall operator. It is thus only necessary to extend Lemmata 1,3,4 and 5 to the operator  $\tilde{h}^{(2)}$  which is obtained from  $h^{BR}$  by including the single-particle second-order potentials  $b_{2m}^{(k)}$ ,  $k = 1, 2$ . We start with the lemmata required for the 'hard part' of the proof.

a) In the formulation of Lemma 1 we simply replace  $h^{BR}$  by  $\tilde{h}^{(2)}$  throughout (and take  $N = 2$ ).

In order to prove  $\|[\tilde{h}^{(2)}, \chi_0] \psi_n\| \leq \frac{c}{n} \|\psi_n\|$  with  $\psi_n \in \mathcal{A}(C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^2)^2$  a Weyl sequence for  $\lambda \in \sigma_{ess}(\tilde{h}^{(2)})$  and  $\chi_0$  from (1.13) with  $\mathbf{x} := (\mathbf{x}_1, \mathbf{x}_2)$ , we have to show in addition to the Brown-Ravenhall case,

$$|(\phi, [b_{2m}^{(1)}, \chi_0] \psi_n)| \leq \frac{c}{n} \|\phi\| \|\psi_n\| \tag{2.12}$$

for all  $\phi \in C_0^\infty(\mathbb{R}^6) \otimes \mathbb{C}^4$ . Due to the symmetry property of  $\psi_n$ , the same bound holds also for  $[b_{2m}^{(2)}, \chi_0]$ . The operator  $b_{2m}^{(1)}$  defined in (2.4) is a sum of terms of the structure  $B(\mathbf{p}_1) \frac{1}{x_1} B_\lambda(\mathbf{p}_1) V_{10,m}^{(1)} B_\mu(\mathbf{p}_1)$  where  $B(\mathbf{p}_1) \in \{A_1, G_1\}$  like for  $b_{1m}^{(1)}$  whereas  $B_\lambda(\mathbf{p}_1), B_\mu(\mathbf{p}_1) \in \{1, \frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}}, \frac{m}{E_{p_1}}, A_1, G_1\}$  are all analytic,

bounded multiplication operators in momentum space. We pick for the sake of demonstration the second term of (2.4) and decompose

$$\begin{aligned}
 [G_1 \frac{1}{x_1} \frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}} V_{10,m}^{(1)} A_1, \chi_0] &= [G_1, \chi_0] p_1 \cdot \frac{1}{p_1 x_1} \frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}} V_{10,m}^{(1)} A_1 \\
 + G_1 \frac{1}{x_1 p_1} \cdot p_1 [\frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}}, \chi_0] V_{10,m}^{(1)} A_1 &+ G_1 \frac{1}{x_1 p_1} \frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}} \cdot p_1 [V_{10,m}^{(1)}, \chi_0] A_1 \\
 + G_1 \frac{1}{x_1 p_1} \frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}} \cdot p_1 V_{10,m}^{(1)} \frac{1}{p_1} \cdot p_1 [A_1, \chi_0]. & \tag{2.13}
 \end{aligned}$$

We will show that the commutators (including the factor  $p_1$ ) are  $\frac{1}{n}$ -bounded and the adjacent factors bounded. The latter is trivial (since also  $\frac{1}{x_1 p_1}$  is bounded,  $\|\frac{1}{x_1 p_1}\| = 2$ , see e.g. [8]) except for the operator  $p_1 V_{10,m}^{(1)} \frac{1}{p_1}$  in the last term. The boundedness of this operator is readily proved by invoking its kernel in momentum space. From (2.1) we have

$$\begin{aligned}
 \|p_1 V_{10,m}^{(1)} \frac{1}{p_1}\| &= 2\pi^2 \left\| \int_0^\infty dt e^{-tE_{p_1}} p_1 \frac{1}{x_1 p_1} e^{-tE_{p_1}} \right\| \\
 &\leq 2\pi^2 \left\| \int_0^\infty dt e^{-tE_{p_1}} p_1 \right\| \cdot \left\| \frac{1}{x_1 p_1} \right\| \cdot \|e^{-tE_{p_1}}\| \leq 4\pi^2 \tag{2.14}
 \end{aligned}$$

where  $\int_0^\infty dt e^{-tE_{p_1}} = 1/E_{p_1}$  has been used.

The commutators  $p_1 [A_1, \chi_0]$  and  $p_1 [G_1, \chi_0]$  have already been dealt with in the context of the Brown-Ravenhall operator.  $p_1 [\frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}}, \chi_0]$  is of the same type, because for any  $B_\lambda$ , one has the estimate  $|B_\lambda(\mathbf{p}_1) - B_\lambda(\mathbf{p}'_1)| = |\mathbf{p}_1 - \mathbf{p}'_1| |\nabla_{\mathbf{p}_1} B_\lambda(\boldsymbol{\xi})| \leq |\mathbf{p}_1 - \mathbf{p}'_1| \frac{c_0}{1+p_1}$  from the mean value theorem, where  $\boldsymbol{\xi}$  is some point between  $\mathbf{p}_1$  and  $\mathbf{p}'_1$ . For the commutator with  $V_{10,m}^{(1)}$  we have

$$\begin{aligned}
 p_1 [V_{10,m}^{(1)}, \chi_0] &= 2\pi^2 \int_0^\infty dt p_1 [e^{-tE_{p_1}}, \chi_0] \frac{1}{x_1} e^{-tE_{p_1}} \\
 + 2\pi^2 \int_0^\infty dt p_1 e^{-tE_{p_1}} \frac{1}{x_1} [e^{-tE_{p_1}}, \chi_0]. & \tag{2.15}
 \end{aligned}$$

The proof of its  $\frac{1}{n}$ -boundedness proceeds with the help of the Lieb and Yau formula [17], derived from the Schwarz inequality (see also [14, Lemma 7]), in momentum space. Explicitly, in the estimate

$$|\langle \hat{\phi}, \widehat{\mathcal{O}} \psi_n \rangle| \leq \left( \int_{\mathbb{R}^6} d\mathbf{p} |\hat{\phi}(\mathbf{p})|^2 I(\mathbf{p}) \right)^{\frac{1}{2}} \left( \int_{\mathbb{R}^6} d\mathbf{p}' |\hat{\psi}_n(\mathbf{p}')|^2 J(\mathbf{p}') \right)^{\frac{1}{2}} \tag{2.16}$$

where  $\mathcal{O} := p_1 [V_{10,m}^{(1)}, \chi_0]$  and  $k_{\mathcal{O}}$  its kernel, one has to show that the integrals  $I$  and  $J$  obey

$$I(\mathbf{p}) := \int_{\mathbb{R}^6} d\mathbf{p}' |k_{\mathcal{O}}(\mathbf{p}, \mathbf{p}')| \frac{f(\mathbf{p})}{f(\mathbf{p}')} \leq \frac{c}{n}$$

$$J(\mathbf{p}') := \int_{\mathbb{R}^6} d\mathbf{p} |k_{\mathcal{O}}(\mathbf{p}, \mathbf{p}')| \frac{f(\mathbf{p}')}{f(\mathbf{p})} \leq \frac{c}{n} \quad (2.17)$$

with some constant  $c$  (independent of  $\mathbf{p}, \mathbf{p}'$ ) for a suitably chosen nonnegative convergence generating function  $f$ .

We use the two-dimensional ( $N = 2$ ) Fourier transform (1.14) of  $\chi_0$  and the momentum representation of  $\frac{1}{x_1}$  to write for the first term in (2.15),

$$\begin{aligned} & \left( \int_0^\infty dt p_1 [e^{-tE_{p_1}}, \chi_0] \widehat{\frac{1}{x_1}} e^{-tE_{p_1}} \varphi \right) (\mathbf{p}_1, \mathbf{p}_2) = \int_{\mathbb{R}^6} d\mathbf{q} d\mathbf{p}'_2 k_1(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}, \mathbf{p}'_2) \hat{\varphi}(\mathbf{q}, \mathbf{p}'_2) \\ k_1(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}, \mathbf{p}'_2) & := \frac{1}{(2\pi)^3} \frac{1}{2\pi^2} p_1 n^6 \int_0^\infty dt \int_{\mathbb{R}^3} d\mathbf{p}'_1 \hat{\chi}_0(n(\mathbf{p}_1 - \mathbf{p}'_1), n(\mathbf{p}_2 - \mathbf{p}'_2)) \\ & \quad \cdot (e^{-tE_{p_1}} - e^{-tE_{p'_1}}) \frac{1}{|\mathbf{p}'_1 - \mathbf{q}|^2} e^{-tE_q}. \end{aligned} \quad (2.18)$$

From the mean value theorem we get

$$|e^{-tE_{p_1}} - e^{-tE_{p'_1}}| = |\mathbf{p}_1 - \mathbf{p}'_1| |te^{-tE_\xi} \frac{\xi}{E_\xi}| \leq |\mathbf{p}_1 - \mathbf{p}'_1| t e^{-tE_\xi} \quad (2.19)$$

with  $\xi = \lambda \mathbf{p}'_1 + (1 - \lambda) \mathbf{p}_1$  for some  $\lambda \in [0, 1]$ . We have to show that the integral over the modulus of the kernel of (2.18), with a suitable convergence generating function  $f$ , is  $\frac{1}{n}$ -bounded. We choose  $f(p) = p$  and make the substitution  $\mathbf{y}_i := n(\mathbf{p}_i - \mathbf{p}'_i)$  for  $\mathbf{p}'_i$ ,  $i = 1, 2$ . Then

$$\begin{aligned} I(\mathbf{p}_1, \mathbf{p}_2) & := \int_{\mathbb{R}^6} d\mathbf{q} d\mathbf{p}'_2 |k_1(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}, \mathbf{p}'_2)| \frac{f(p_1)}{f(q)} \\ & \leq \frac{1}{(2\pi)^4 \pi} p_1 \int_0^\infty dt \int_{\mathbb{R}^3} d\mathbf{q} \int_{\mathbb{R}^6} d\mathbf{y}_1 d\mathbf{y}_2 |\hat{\chi}_0(\mathbf{y}_1, \mathbf{y}_2)| \\ & \quad \cdot \frac{y_1}{n} t e^{-tE_\xi} \frac{1}{|\mathbf{q} - (\mathbf{p}_1 - \mathbf{y}_1/n)|^2} e^{-tE_q} \cdot \frac{p_1}{q}. \end{aligned} \quad (2.20)$$

The  $t$ -integral can be carried out,  $\int_0^\infty dt t e^{-(E_\xi + E_q)} = (E_\xi + E_q)^{-2}$  with  $\xi = \mathbf{p}_1 - \frac{\lambda}{n} \mathbf{y}_1$ . Define  $\mathbf{q}_1 := \mathbf{p}_1 - \mathbf{y}_1/n$  and consider

$$S := p_1^2 \int_{\mathbb{R}^3} d\mathbf{q} \frac{1}{|\mathbf{q} - \mathbf{q}_1|^2} \frac{1}{q} \frac{1}{(E_\xi + E_q)^2}. \quad (2.21)$$

Estimating the last factor by  $\frac{1}{E_\xi} \cdot \frac{1}{q}$  and performing the angular integration, one obtains

$$S \leq p_1^2 \frac{2\pi}{q_1} \frac{1}{E_\xi} \int_0^\infty \frac{dq}{q} \ln \left| \frac{q + q_1}{q - q_1} \right| = \pi^3 \frac{p_1}{|\mathbf{p}_1 - \mathbf{y}_1/n|} \frac{p_1}{\sqrt{(\mathbf{p}_1 - \frac{\lambda}{n} \mathbf{y}_1)^2 + m^2}}. \quad (2.22)$$

Insertion into (2.20) gives

$$I(\mathbf{p}_1, \mathbf{p}_2) \leq \frac{1}{(4\pi)^2} \frac{1}{n} \int_{\mathbb{R}^6} d\mathbf{y}_1 d\mathbf{y}_2 |\hat{\chi}_0(\mathbf{y}_1, \mathbf{y}_2)| y_1 \frac{p_1}{|\mathbf{p}_1 - \mathbf{y}_1/n|} \frac{p_1}{\sqrt{(\mathbf{p}_1 - \frac{\lambda}{n}\mathbf{y}_1)^2 + m^2}} \leq \frac{c}{n} \tag{2.23}$$

because the singularity at  $\mathbf{y}_1 = n\mathbf{p}_1$  is integrable and the integral is finite for all  $p_1 \geq 0$  due to  $\hat{\chi}_0 \in \mathcal{S}(\mathbb{R}^6)$ . Since the kernel  $k_1$  is not symmetric in  $\mathbf{p}_1, \mathbf{q}$ , the estimate of  $J(\mathbf{q}, \mathbf{p}'_2) := \int_{\mathbb{R}^6} d\mathbf{p}_1 d\mathbf{p}_2 |k_1(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}, \mathbf{p}'_2)| \frac{f(q)}{f(p_1)}$  is needed too. The  $\frac{1}{n}$ -boundedness of  $J(\mathbf{q}, \mathbf{p}'_2)$  can be shown along the same lines, using  $(E_{\xi'} + E_q)^{-2} \leq \xi'^{-2}$  with  $\xi' := \mathbf{p}'_1 + \lambda(\mathbf{p}_1 - \mathbf{p}'_1)$ .

We still have to estimate the second term in (2.15). Its kernel is

$$k_2(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}, \mathbf{p}'_2) := \frac{1}{(2\pi)^3} \frac{1}{2\pi^2} p_1 n^6 \int_0^\infty dt e^{-tE_{p_1}} \int_{\mathbb{R}^3} d\mathbf{p}'_1 \frac{1}{|\mathbf{p}_1 - \mathbf{p}'_1|^2} \hat{\chi}_0(n(\mathbf{p}'_1 - \mathbf{q}), n(\mathbf{p}_2 - \mathbf{p}'_2)) (e^{-tE_{p'_1}} - e^{-tE_q}). \tag{2.24}$$

With (2.19) the  $t$ -integral can be carried out as before. Making the substitution  $\mathbf{y}_1 := n(\mathbf{p}'_1 - \mathbf{q})$ ,  $\mathbf{y}_2 := n(\mathbf{p}_2 - \mathbf{p}'_2)$  for  $\mathbf{q}$  and  $\mathbf{p}'_2$ , respectively, one gets with the choice  $f(p) = p^{\frac{1}{2}}$ ,

$$\begin{aligned} \tilde{I}(\mathbf{p}_1, \mathbf{p}_2) &:= \int_{\mathbb{R}^6} d\mathbf{q} d\mathbf{p}'_2 |k_2(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}, \mathbf{p}'_2)| \frac{f(p_1)}{f(q)} \tag{2.25} \\ &\leq \frac{1}{(2\pi)^4 \pi} p_1 \int_{\mathbb{R}^6} d\mathbf{y}_1 d\mathbf{y}_2 |\hat{\chi}_0(\mathbf{y}_1, \mathbf{y}_2)| \int_{\mathbb{R}^3} d\mathbf{p}'_1 \frac{1}{|\mathbf{p}_1 - \mathbf{p}'_1|^2} \frac{y_1}{n} \frac{1}{(E_{p_1} + E_{\tilde{\xi}})^2} \cdot \frac{p_1^{\frac{1}{2}}}{|\mathbf{p}'_1 - \frac{\mathbf{y}_1}{n}|^{\frac{1}{2}}} \end{aligned}$$

with  $\tilde{\xi} := \lambda\mathbf{q} + (1-\lambda)\mathbf{p}'_1 = \mathbf{p}'_1 - \frac{\lambda}{n}\mathbf{y}_1$ . We estimate  $(E_{p_1} + E_{\tilde{\xi}})^{-2} \leq p_1^{-\frac{1}{2}} E_{\tilde{\xi}}^{-\frac{3}{2}}$ . Then the integral over  $\mathbf{p}'_1$  reduces to

$$\tilde{S} := p_1 \int_{\mathbb{R}^3} d\mathbf{p}'_1 \frac{1}{|\mathbf{p}_1 - \mathbf{p}'_1|^2} \frac{1}{|\mathbf{p}'_1 - \frac{\mathbf{y}_1}{n}|^{\frac{1}{2}}} \frac{1}{[(\mathbf{p}'_1 - \frac{\lambda}{n}\mathbf{y}_1)^2 + m^2]^{\frac{3}{4}}}. \tag{2.26}$$

Even when the two singularities coincide (for  $\mathbf{y}_1 = n\mathbf{p}_1$ ), they are integrable. Since the integrand behaves like  $p_1'^{-2}$  for  $p_1' \rightarrow \infty$ ,  $\tilde{S}$  is finite for all  $0 \leq p_1 < \infty$ . It remains to estimate  $\tilde{S}$  for  $p_1 \rightarrow \infty$ . We substitute  $p_1\mathbf{x} := \mathbf{p}'_1 - \mathbf{p}_1$ , such that with  $\mathbf{e}_{p_1} := \mathbf{p}_1/p_1$ ,

$$\begin{aligned} \tilde{S} &= \int_{\mathbb{R}^3} \frac{d\mathbf{x}}{x^2} \frac{1}{|\mathbf{x} + \mathbf{e}_{p_1} - \frac{\mathbf{y}_1}{np_1}|^{\frac{1}{2}}} \frac{1}{[(\mathbf{x} + \mathbf{e}_{p_1} - \frac{\lambda}{np_1}\mathbf{y}_1)^2 + \frac{m^2}{p_1^2}]^{\frac{3}{4}}} \\ &\longrightarrow \int_{\mathbb{R}^3} \frac{d\mathbf{x}}{x^2} \frac{1}{|\mathbf{x} + \mathbf{e}_{p_1}|^2} = \pi^3 \quad \text{as } p_1 \rightarrow \infty. \tag{2.27} \end{aligned}$$

Therefore,  $\tilde{I}$  is  $\frac{1}{n}$ -bounded for all  $p_1 \geq 0$ . It is easy to prove that also  $\tilde{J}(\mathbf{q}, \mathbf{p}'_2) := \int_{\mathbb{R}^6} d\mathbf{p}_1 d\mathbf{p}_2 |k_2(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}, \mathbf{p}'_2)| \frac{q^{\frac{1}{2}}}{p_1^{\frac{1}{2}}}$  is  $\frac{1}{n}$ -bounded, using the estimate  $(E_{p_1} + E_{|\mathbf{q}+\lambda(\mathbf{p}'_1-\mathbf{q})|})^{-2} \leq p_1^{-2}$ .

Collecting results, this shows the  $\frac{1}{n}$ -boundedness of  $p_1[V_{10,m}^{(1)}, \chi_0]$ . With the same tools, the  $\frac{1}{n}$ -boundedness of the commutator of  $\chi_0$  with the remaining contributions from (2.4) to  $b_{2m}^{(1)}$  is established.

The second item of Lemma 1, the normalizability of the sequence  $\varphi_n := (1 - \chi_0)\psi_n$ , follows immediately from the proof concerning the Brown-Ravenhall operator, because of the relative form boundedness of the total potential of  $\tilde{h}^{(2)}$  with form bound smaller than one for  $\gamma < \gamma_{BR}$  ( see [13] and Lemma 7).

b) In the formulation of Lemma 3, the only change is again the replacement of  $h^{BR}$  with  $\tilde{h}^{(2)}$  (and  $N = 2$ ).

We consider the case  $j = 1$  where  $r_1 = b_{1m}^{(1)} + b_{2m}^{(1)} + v^{(12)}$ , and we have to show in addition to the Brown-Ravenhall case that

$$|(\phi_1\varphi, b_{2m}^{(1)}\phi_1\varphi)| \leq \frac{c}{R} \|\varphi\|^2 \tag{2.28}$$

provided  $\varphi \in \mathcal{A}(C_0^\infty(\mathbb{R}^6 \setminus B_R(0)) \otimes \mathbb{C}^4)$  and  $R > 1$ .

We note that every summand of  $b_{2m}^{(1)}$  in (2.4) is of the form  $B_1 \frac{1}{x_1} W_1$  or  $W_1 \frac{1}{x_1} B_1$  where  $B_1$  is a bounded multiplication operator in momentum space, while  $W_1$  is a bounded integral operator. For operators of the first type we take the smooth auxiliary function  $\chi_1(\frac{\mathbf{x}_1}{R})$  from (1.17) which is unity on the support of  $\phi_1\varphi$  and decompose

$$(\chi_1\phi_1\varphi, B_1 \frac{1}{x_1} W_1 \phi_1\varphi) = (\phi_1\varphi, B_1\chi_1 \frac{1}{x_1} W_1 \phi_1\varphi) + (\phi_1\varphi, [\chi_1, B_1] \frac{1}{x_1} W_1 \phi_1\varphi). \tag{2.29}$$

Since  $\text{supp } \chi_1 \subset \mathbb{R}^3 \setminus B_{CR/2}(0)$  we have

$$\begin{aligned} |(B_1\phi_1\varphi, \chi_1 \frac{1}{x_1} W_1 \phi_1\varphi)| &\leq \frac{2}{CR} \int_{\mathbb{R}^6} d\mathbf{x}_1 d\mathbf{x}_2 |(B_1\phi_1\varphi)(\mathbf{x}_1, \mathbf{x}_2)| |\chi_1|(W_1\phi_1\varphi)(\mathbf{x}_1, \mathbf{x}_2)| \\ &\leq \frac{2}{CR} \|B_1\| \|\varphi\| \|W_1\| \|\varphi\| \leq \frac{c_0}{R} \|\varphi\|^2. \end{aligned} \tag{2.30}$$

For the second contribution to (2.29), we have to estimate  $[\chi_{1,0}, B_1]p_1$  with  $\chi_{1,0} := 1 - \chi_1$  in momentum space. Since  $B_1 \in \{A_1, G_1\}$  we use the relation  $|(\tilde{\varphi}, [\chi_{1,0}, B_1]p_1\tilde{\psi})| = |(\tilde{\psi}, p_1[B_1, \chi_{1,0}]\tilde{\varphi})|$  (for suitable  $\tilde{\varphi}, \tilde{\psi}$ ), the uniform  $\frac{1}{R}$ -boundedness of which has already been proven in the context of the Brown-Ravenhall case. The second operator,  $W_1 \frac{1}{x_1} B_1$  is treated in the same way, using  $W_1 \frac{1}{x_1} B_1 \chi_1 \phi_1\varphi = W_1 \frac{1}{x_1} \chi_1 B_1 \phi_1\varphi + W_1 \frac{1}{x_1} [B_1, \chi_1] \phi_1\varphi$ .

In the case  $j = 0$  we have  $r_0 = \sum_{k=1}^2 (b_{1m}^{(k)} + b_{2m}^{(k)})$ , and since  $\text{supp } \phi_0$  requires  $x_1 \geq Cx$  as well as  $x_2 \geq Cx$ ,  $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2)$ , the auxiliary function can be

taken from (1.17) for  $k = 1$  or  $k = 2$ . The further proof of the lemma is identical to the one for  $j = 1$ .

c) Lemma 4 (formulated for  $\tilde{h}^{(2)}$  in place of  $h^{BR}$ ) which is needed for the localization formula, has to be supplemented with the following estimate

$$(d) \quad |(\phi_j \varphi, [b_{2m}^{(k)}, \phi_j] \varphi)| \leq \frac{c}{R} \|\varphi\|^2 \tag{2.31}$$

for  $\varphi \in \mathcal{A}(C_0^\infty(\mathbb{R}^6 \setminus B_R(0)) \otimes \mathbb{C}^4)$  and  $R > 2$ .

The proof is carried out in coordinate space as are the proofs of the Brown-Ravenhall items of Lemma 4. We split the commutator in the same way as in the proof of Lemma 1. In order to show how to proceed, we pick again the second term of (2.4), take  $k = 1$  and decompose

$$\begin{aligned} [G_1 \frac{1}{x_1} \frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}} V_{10,m}^{(1)} A_1, \phi_j] &= [G_1, \phi_j] \frac{1}{x_1} \cdot \frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}} V_{10,m}^{(1)} A_1 \\ + G_1 \frac{1}{x_1} [\frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}}, \phi_j] V_{10,m}^{(1)} A_1 &+ G_1 \frac{1}{x_1} \frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}} x_1 \cdot \frac{1}{x_1} [V_{10,m}^{(1)}, \phi_j] A_1 \\ &+ G_1 \frac{1}{x_1} \frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}} V_{10,m}^{(1)} x_1 \cdot \frac{1}{x_1} [A_1, \phi_j]. \end{aligned} \tag{2.32}$$

We have to prove the  $\frac{1}{R}$ -boundedness of the commutators (including the factor  $\frac{1}{x_1}$ ) and to assure the boundedness of the adjacent operators. The commutators with  $G_1$  and  $A_1$  have already been dealt with in the Brown-Ravenhall case. As concerns  $[\frac{\sigma^{(1)} \mathbf{p}_1}{E_{p_1}}, \phi_j] \frac{1}{x_1}$ , we have to show that its kernel obeys the estimate

$$|\check{k}_{\sigma^{(1)} \mathbf{p}_1 \frac{1}{E_{p_1}}}(\mathbf{x}_1, \mathbf{x}'_1)| \leq \frac{c}{|\mathbf{x}_1 - \mathbf{x}'_1|^3} \tag{2.33}$$

with some constant  $c$ . When dealing with the Brown-Ravenhall operator, we have shown the corresponding estimate for the kernel of the operator  $\sigma^{(1)} \mathbf{p}_1 g(p_1)$  with  $g(p_1) = [2(p_1^2 + m^2 + m\sqrt{p_1^2 + m^2})]^{-\frac{1}{2}}$ . Replacing  $g(p_1)$  with  $(p_1^2 + m^2)^{-\frac{1}{2}}$  does neither change the analyticity property of the kernel nor its behaviour as  $|\mathbf{x}_1 - \mathbf{x}'_1|$  tends to 0 or infinity, from which (2.33) is established [14].

For the further proof of the  $\frac{1}{R}$ -boundedness of the commutator, we can substitute  $\phi_j$  with  $\phi_j \chi$  where  $\chi(\frac{\mathbf{x}}{R})$  is defined in (1.20) with  $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2)$  (see the discussion below (1.20)). Thus we can use the estimate (1.21) (for  $k = 1$  and  $N = 2$ ) derived from the mean value theorem and mimic the proof of the two-electron Brown-Ravenhall case.

For the treatment of the remaining commutator,  $[V_{10,m}^{(1)}, \phi_j \chi] \frac{1}{x_1}$ , we set  $\psi_j := \phi_j \chi$  and decompose

$$[V_{10,m}^{(1)}, \psi_j] \frac{1}{x_1} = [V_{10,m}^{(1)} \frac{1}{x_1}, \psi_j] \tag{2.34}$$

$$= 2\pi^2 \int_0^\infty dt [e^{-tE_{p_1}}, \psi_j] \frac{1}{x_1} e^{-tE_{p_1}} \frac{1}{x_1} + 2\pi^2 \int_0^\infty dt e^{-tE_{p_1}} \frac{1}{x_1} [e^{-tE_{p_1}}, \psi_j] \frac{1}{x_1}.$$

The kernel of  $e^{-tE_{p_1}}$  in coordinate space is given by [17]

$$\check{k}_{e^{-tE_{p_1}}}(\mathbf{x}_1, \mathbf{x}'_1, t) = \check{k}_{e^{-tE_{p_1}}}(\tilde{\mathbf{x}}, t) = \frac{t}{2\pi^2} \frac{m^2}{\tilde{x}^2 + t^2} K_2(m\sqrt{\tilde{x}^2 + t^2}) \quad (2.35)$$

where  $K_2$  is a modified Bessel function of the second kind and  $\tilde{\mathbf{x}} := \mathbf{x}_1 - \mathbf{x}'_1$ . Making use of the analyticity of  $K_2(z)$  for  $z > 0$  and its behaviour  $K_2(z) \sim \frac{2}{z^2}$  for  $z \rightarrow 0$  and  $K_2(z) \sim \sqrt{\frac{\pi}{2z}} e^{-z}$  for  $z \rightarrow \infty$  [1, p.377] we have

$$|K_2(z)| \leq \frac{2c_1}{z^2} \quad (2.36)$$

and therefore we can estimate  $\check{k}_{e^{-tE_{p_1}}}$  by the corresponding kernel for  $m = 0$ ,

$$|\check{k}_{e^{-tE_{p_1}}}(\tilde{\mathbf{x}}, t)| \leq \frac{t}{\pi^2} \frac{c_1}{(\tilde{x}^2 + t^2)^2} = c_1 \check{k}_{e^{-tE_{p_1}}}(\tilde{\mathbf{x}}, t). \quad (2.37)$$

Thus we obtain for the kernel of the second contribution to (2.34), using (2.37) and (1.21),

$$\begin{aligned} S_0 &:= \left| \int_0^\infty dt \check{k}_{e^{-tE_{p_1}} \frac{1}{x_1} [e^{-tE_{p_1}}, \psi_j] \frac{1}{x_1}}(\mathbf{x}_1, \mathbf{y}_1, \mathbf{x}_2) \right| \quad (2.38) \\ &= \left| \int_0^\infty dt \int_{\mathbb{R}^3} d\mathbf{x}'_1 \frac{t}{2\pi^2} \frac{m^2}{(\mathbf{x}_1 - \mathbf{x}'_1)^2 + t^2} K_2(m\sqrt{(\mathbf{x}_1 - \mathbf{x}'_1)^2 + t^2}) \frac{1}{x'_1} \right. \\ &\quad \left. \cdot \frac{t}{2\pi^2} \frac{m^2}{(\mathbf{x}'_1 - \mathbf{y}_1)^2 + t^2} K_2(m\sqrt{(\mathbf{x}'_1 - \mathbf{y}_1)^2 + t^2}) \frac{1}{y_1} (\psi_j(\mathbf{y}_1, \mathbf{x}_2) - \psi_j(\mathbf{x}'_1, \mathbf{x}_2)) \right| \\ &\leq \frac{c_1^2}{\pi^4} \int_0^\infty t^2 dt \int_{\mathbb{R}^3} d\mathbf{x}'_1 \frac{1}{[(\mathbf{x}_1 - \mathbf{x}'_1)^2 + t^2]^2} \frac{1}{x'_1} \frac{1}{[(\mathbf{x}'_1 - \mathbf{y}_1)^2 + t^2]^2} \frac{1}{y_1} \cdot |\mathbf{x}'_1 - \mathbf{y}_1| \frac{c_0}{R}. \end{aligned}$$

With the help of the estimate  $\frac{1}{[(\mathbf{x}'_1 - \mathbf{y}_1)^2 + t^2]^2} \leq \frac{1}{t} \frac{1}{|\mathbf{x}'_1 - \mathbf{y}_1|^3}$ , the  $t$ -integral can be carried out,

$$\int_0^\infty dt \frac{t}{[(\mathbf{x}_1 - \mathbf{x}'_1)^2 + t^2]^2} = \frac{1}{2|\mathbf{x}_1 - \mathbf{x}'_1|^2}. \quad (2.39)$$

According to the Lieb and Yau formula (2.16) in coordinate space, the  $\frac{1}{R}$ -boundedness of  $S_0$  integrated over  $\mathbf{y}_1$ , respectively over  $\mathbf{x}_1$ , with a suitably chosen convergence generating function  $f$ , has to be shown (in analogy to (2.17)).

With the choice  $f(x) = x^\alpha$  and (2.39) we have

$$I(\mathbf{x}_1) := \int_{\mathbb{R}^3} d\mathbf{y}_1 S_0 \frac{f(x_1)}{f(y_1)}$$

$$\leq \frac{\tilde{c}}{R} \int_{\mathbb{R}^3} d\mathbf{x}'_1 \frac{1}{|\mathbf{x}_1 - \mathbf{x}'_1|^2} \frac{1}{x'_1} \int_{\mathbb{R}^3} d\mathbf{y}_1 \frac{1}{y_1} \frac{1}{|\mathbf{x}'_1 - \mathbf{y}_1|^2} \cdot \frac{x_1^\alpha}{y_1^\alpha}. \tag{2.40}$$

With the substitutions  $\mathbf{y}_1 =: x'_1 \mathbf{z}$  and then  $\mathbf{x}'_1 =: x_1 \boldsymbol{\xi}$  the two integrals separate such that (with  $\mathbf{e}_x := \mathbf{x}/x$ )

$$I(\mathbf{x}_1) \leq \frac{\tilde{c}}{R} \int_{\mathbb{R}^3} \frac{d\boldsymbol{\xi}}{\xi^{1+\alpha}} \frac{1}{|\mathbf{e}_{x_1} - \boldsymbol{\xi}|^2} \cdot \int_{\mathbb{R}^3} \frac{d\mathbf{z}}{z^{1+\alpha}} \frac{1}{|\mathbf{e}_{x'_1} - \mathbf{z}|^2} \leq \frac{C}{R} \tag{2.41}$$

if  $0 < \alpha < 2$  [3]. In the same way it is shown that  $J(\mathbf{y}_1) := \int_{\mathbb{R}^3} d\mathbf{x}_1 S_0 \frac{y_1^\alpha}{x_1^\alpha} \leq \frac{C}{R}$  for  $1 < \alpha < 3$ . Thus  $\alpha = 3/2$  assures the  $1/R$ -boundedness of  $I$  and  $J$ . The first contribution to (2.34) is treated along the same lines. This proves the  $1/R$ -boundedness of  $[V_{10,m}^{(1)}, \psi_j] \frac{1}{x_1}$ .

Finally the boundedness of the two operators occurring in (2.32),  $\frac{1}{x_1} \frac{\boldsymbol{\sigma}^{(1)} \mathbf{p}_1}{E_{p_1}} x_1$  and  $\frac{1}{x_1} V_{10,m}^{(1)} x_1$ , has to be shown. We use the fact that for any bounded operator  $\mathcal{O}$ ,  $\frac{1}{x_1} \mathcal{O} x_1 = \frac{1}{x_1} [\mathcal{O}, x_1] + \mathcal{O}$ , such that for the first operator, only the boundedness of  $\frac{1}{x_1} [\frac{\boldsymbol{\sigma}^{(1)} \mathbf{p}_1}{E_{p_1}}, x_1]$  has to be established. We use the estimate (2.33) to write

$$\begin{aligned} & \left| \check{k}_{\frac{1}{x_1} [\frac{\boldsymbol{\sigma}^{(1)} \mathbf{p}_1}{E_{p_1}}, x_1]}(\mathbf{x}_1, \mathbf{x}'_1) \right| \\ &= \left| \frac{1}{x_1} \check{k}_{\frac{\boldsymbol{\sigma}^{(1)} \mathbf{p}_1}{E_{p_1}}}(\mathbf{x}_1, \mathbf{x}'_1) \cdot (x_1 - x'_1) \right| \leq \frac{\tilde{c}}{x_1} \frac{1}{|\mathbf{x}_1 - \mathbf{x}'_1|^2} \end{aligned} \tag{2.42}$$

and with the choice  $f(x) = x^{3/2}$ , (2.42) multiplied by  $f(x_1)/f(x'_1)$  and integrated over  $d\mathbf{x}'_1$ , respective multiplied by  $f(x'_1)/f(x_1)$  and integrated over  $d\mathbf{x}_1$ , is finite. This proves the desired boundedness.

Concerning the operator  $\frac{1}{x_1} V_{10,m}^{(1)} x_1$  we decompose

$$\frac{1}{x_1} V_{10,m}^{(1)} x_1 = 2\pi^2 \int_0^\infty dt \frac{1}{x_1} e^{-tE_{p_1}} \frac{1}{x_1} \{ [e^{-tE_{p_1}}, x_1] + x_1 e^{-tE_{p_1}} \}. \tag{2.43}$$

In the second contribution the  $t$ -integral can be carried out,  $\int_0^\infty dt \frac{1}{x_1} e^{-2tE_{p_1}} = \frac{1}{2x_1 E_{p_1}}$  which is a bounded operator. For the first contribution, we can again use the estimate (2.36) for the Bessel function together with the estimate for the  $t$ -dependence, resulting in (2.39), such that

$$\begin{aligned} \tilde{S}_0 &:= \left| \int_0^\infty dt \check{k}_{\frac{1}{x_1} e^{-tE_{p_1}} \frac{1}{x_1} [e^{-tE_{p_1}}, x_1]}(\mathbf{x}_1, \mathbf{y}_1) \right| \\ &= \left| \int_0^\infty dt \frac{1}{x_1} \int_{\mathbb{R}^3} d\mathbf{x}'_1 \frac{t}{2\pi^2} \frac{m^2}{|\mathbf{x}_1 - \mathbf{x}'_1|^2 + t^2} K_2(m\sqrt{(\mathbf{x}_1 - \mathbf{x}'_1)^2 + t^2}) \frac{1}{x'_1} \right| \end{aligned} \tag{2.44}$$

$$\begin{aligned} & \cdot \frac{t}{2\pi^2} \frac{m^2}{(\mathbf{x}'_1 - \mathbf{y}_1)^2 + t^2} K_2(m\sqrt{(\mathbf{x}'_1 - \mathbf{y}_1)^2 + t^2}) (y_1 - x'_1) \Big| \\ & \leq \tilde{c}_0 \frac{1}{x_1} \int_{\mathbb{R}^3} d\mathbf{x}'_1 \frac{1}{|\mathbf{x}_1 - \mathbf{x}'_1|^2} \frac{1}{x'_1} \frac{1}{|\mathbf{x}'_1 - \mathbf{y}_1|^2}. \end{aligned}$$

With  $\alpha = 3/2$ , in the same way as shown in the step from (2.40) to (2.41), one obtains  $\tilde{I}(\mathbf{x}_1) := \int_{\mathbb{R}^3} d\mathbf{y}_1 \tilde{S}_0 \frac{x_1^\alpha}{y_1^\alpha} \leq c$  and  $\tilde{J}(\mathbf{y}_1) := \int_{\mathbb{R}^3} d\mathbf{x}_1 \tilde{S}_0 \frac{y_1^\alpha}{x_1^\alpha} \leq c$ . Thus the boundedness of  $\frac{1}{x_1} V_{10,m}^{(1)} x_1$  is shown.

In the remaining contributions to  $[b_{2m}^{(1)}, \phi_j \chi]$  the terms not treated so far are  $[\frac{m}{E_{p_1}}, \phi_j \chi] \frac{1}{x_1}$ , the  $\frac{1}{R}$ -boundedness of which follows from the estimate  $|\check{k}_{\frac{m}{E_{p_1}}}(\mathbf{x}_1, \mathbf{x}'_1)| \leq c/|\mathbf{x}_1 - \mathbf{x}'_1|^3$  (which is proven in the same way as the corresponding Brown-Ravenhall estimate for  $\tilde{g}(p_1) := \frac{m}{\sqrt{2}} (E_{p_1} + \sqrt{E_{p_1}^2 + mE_{p_1}})^{-1}$  in place of  $m/E_{p_1}$  [14]). The boundedness of the additional term  $\frac{1}{x_1} \frac{m}{E_{p_1}} x_1$  (respective  $\frac{1}{x_1} [\frac{m}{E_{p_1}}, x_1]$ ) follows from (2.42) formulated for  $\check{k}_{\frac{m}{E_{p_1}}}$ . This completes the proof of Lemma 4.

We now turn to the 'easy part' of the HVZ theorem, where we have to assure that  $[\Sigma_0, \infty) \subset \sigma_{ess}(\tilde{h}^{(2)})$ . We use the method of proof applied to the multi-particle Brown-Ravenhall operator (see section 1 (b)). The proof of continuity of  $\sigma(T + a_j)$  for  $j \in \{0, \dots, N\}$  with  $a_j$  from (2.5) does not depend on the choice of the single-particle potential and hence also holds true for the Jansen-Hess operator. With  $T_{\mathbf{a}}$  from (1.25) for  $N = 2$  and  $\varphi_n \in C_0^\infty(\mathbb{R}^6) \otimes \mathbb{C}^4$  a defining sequence for  $\lambda \in \sigma(T + a_j)$  we have (according to (1.26)) to show that  $\|r_j T_{\mathbf{a}} \varphi_n\| < \epsilon$  for  $n$  and  $a$  sufficiently large, where  $r_j$  now includes the terms  $b_{2m}^{(k)}$  with  $k \notin C_{1j}$ .

(d) Lemma 5 has therefore to be supplemented with the conjecture

$$\|b_{2m}^{(k)} \varphi\| \leq \frac{c}{R} \|\varphi\| \tag{2.45}$$

where  $\varphi \in C_0^\infty(\Omega) \otimes \mathbb{C}^{2l}$  with  $\Omega := \{\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_l) \in \mathbb{R}^{3l} : x_i > R \ \forall i = 1, \dots, l\}$ ,  $R > 1$  and  $k \in \{1, \dots, l\}$  where  $l$  is the number of electrons in cluster  $C_{2j}$ . The domain  $\Omega$  allows for the introduction of the auxiliary function  $\chi$  from (1.31) which is unity on the support of  $\varphi$ .

As discussed in the proof of Lemma 3,  $b_{2m}^{(k)}$  consists (for  $k = 1$ ) of terms like  $W_1 \frac{1}{x_1} B_1$  (and its Hermitean conjugate), such that the idea of (2.29) can be used,

$$|(\phi, W_1 \frac{1}{x_1} B_1 \varphi)| \leq |(W_1 \phi, \frac{1}{x_1} \chi B_1 \varphi)| + |(W_1 \phi, \frac{1}{x_1} [\chi, B_1] \varphi)|. \tag{2.46}$$

Therefore, the proof of Lemma 3 establishes the validity of (2.45), too. Thus the proof of Theorem 2 is complete. □

We remark that the two-particle potentials of  $\tilde{h}^{(2)}$  coincide with those of  $h^{BR}$  and hence are nonnegative. Therefore, as demonstrated in section 1 (below (1.9)),  $j = 0$  (corresponding to the cluster decomposition where the nucleus is separated from all electrons) can be omitted in the determination of  $\Sigma_0$ . Thus the infimum of the essential spectrum of  $h^{(2)}$  is given by the first ionization threshold (i.e. the infimum of the spectrum of the operator describing an ion with one electron less) increased by the electron's rest energy  $m$ .

### 3 THE MULTIPARTICLE JANSEN-HESS OPERATOR

Let

$$\begin{aligned}
 H_N^{(2)} &:= H^{BR} + \Lambda_{+,N} \left( \sum_{k=1}^N B_{2m}^{(k)} + \sum_{k>l=1}^N C^{(kl)} \right) \Lambda_{+,N} \\
 &=: \tilde{H}_N^{(2)} + \Lambda_{+,N} \sum_{k>l=1}^N C^{(kl)} \Lambda_{+,N}
 \end{aligned}
 \tag{3.1}$$

with  $H^{BR}$  from (1.1) and the second-order potentials from (2.1) and (2.2). According to section 1, the proofs of the required lemmata to assure the HVZ theorem for  $\tilde{H}_N^{(2)}$  are easily generalized to the  $N$ -electron case (with the exception of Lemma 1). For Lemma 1 to hold, we have to establish the form boundedness of the total potential  $\tilde{W}_0$  of  $\tilde{H}_N^{(2)}$  with respect to the multiparticle kinetic energy  $T_0$ . We can prove (see Appendix A)

LEMMA 7. *Let  $\tilde{H}_N^{(2)} =: T_0 + \tilde{W}_0$  be (as defined in (3.1) with  $T_0 := \Lambda_{+,N} \sum_{k=1}^N D_0^{(k)} \Lambda_{+,N}$ ) the  $N$ -electron Jansen-Hess operator without the second-order two-electron interaction terms, acting on  $\mathcal{A}(H_1(\mathbb{R}^3) \otimes \mathbb{C}^4)^N$ . Then  $\tilde{W}_0$  is relatively form bounded with respect to the kinetic energy operator  $T_0$ ,*

$$|(\psi, \tilde{W}_0 \psi)| \leq c_1 (\psi, T_0 \psi) + C_1 (\psi, \psi) \tag{3.2}$$

with  $c_1 < 1$  for  $\gamma < \gamma_{BR}$  irrespective of the electron number  $N$  (for  $N \leq Z$ ).

We remark that the relative form boundedness of the total potential  $W_0 := H_N^{(2)} - T_0$  holds only for a smaller critical  $\gamma$ . Using the estimate  $|(\psi_+, \sum_{k>l=1}^N C^{(kl)} \psi_+)| \leq \gamma \frac{e^2 \pi^2}{2} \frac{N-1}{2} (\psi, T_0 \psi)$  with  $\psi_+ := \Lambda_{+,N} \psi$  [13], we found  $\gamma < 0.454$  ( $Z \leq 62$ ) for  $N = Z$ .

The proof of Lemma 1 for the  $N$ -electron operator  $\tilde{H}_N^{(2)}$  is then done in the same way as for the Brown-Ravenhall operator in section 1 (using the estimates for the second-order single-particle interaction from section 2 (a)).

For the proof of Proposition 1 formulated for the  $N$ -electron case we note that the resolvent  $R_{N,\mu} := (H_N^{(2)} + \mu)^{-1} - (\tilde{H}_N^{(2)} + \mu)^{-1}$  can be written as a finite sum of compact operators of the type (2.10). In place of  $W_2$ , we have

$W_{kl} := (T + \mu)^{-1}C^{(kl)}(T + \mu)^{-1}$  with the  $N$ -particle kinetic energy  $T$ . Since, however,  $(T + \mu)^{-1} \leq (T^{(k)} + T^{(l)} + \mu)^{-1}$ , the compactness proof for  $W_{kl}$  can be copied from the  $N = 2$  case. In addition, we have to assure the relative operator boundedness of the total potential of  $H_N^{(2)}$ :

LEMMA 8. *Let  $H_N^{(2)} =: T_0 + W_0$  be the  $N$ -electron Jansen-Hess operator. For  $\gamma < \gamma_1$  the total potential  $W_0$  is bounded by the kinetic energy operator,*

$$\|W_0 \psi\| \leq c_0 \|T_0 \psi\| \tag{3.3}$$

with  $c_0 < 1$ . For  $N = Z$  (and  $m = 0$ ),  $\gamma_1 = 0.285$  ( $Z \leq 39$ ).

The proof is given in Appendix B. A consequence of this proof is the relative boundedness of the total potential of  $\tilde{H}_N^{(2)}$  (with bound  $< 1$ ) for  $\gamma < \gamma_1$ . We note that the critical potential strength may well be improved by using more refined techniques for the estimate of  $W_0\psi$  in the case of large  $N$ .

Collecting results, we have shown that the HVZ theorem holds also for the  $N$ -electron Jansen-Hess operator, provided  $\gamma$  is below a critical potential strength ( $\gamma < 0.285$  if  $N = Z$ ).

APPENDIX A (PROOF OF LEMMA 7)

When showing the relative form boundedness of the potential  $\tilde{W}_0$ , we can disregard the projectors  $\Lambda_{+,N}$  in (1.1) and (3.1). In fact, define the potential  $\tilde{W}$  by  $\tilde{H}_N^{(2)} = T_0 + \tilde{W} =: \Lambda_{+,N}(\sum_{k=1}^N D_0^{(k)} + \tilde{W})\Lambda_{+,N}$ . Assume we prove for  $\psi_+ := \Lambda_{+,N}\psi \in \Lambda_{+,N}(\mathcal{A}(H_1(\mathbb{R}^3) \otimes \mathbb{C}^4)^N)$  an  $N$ -particle function in the positive spectral subspace and  $T = E_{p_1} + \dots + E_{p_N}$ ,

$$|(\psi_+, \tilde{W}\psi_+)| \leq c_1 (\psi_+, T\psi_+) + C_1 (\psi_+, \psi_+) \tag{A.1}$$

with constants  $c_1 < 1$  and  $C_1 \geq 0$ . Then we get

$$(\psi, \tilde{W}_0\psi) = (\psi, \Lambda_{+,N}\tilde{W}\Lambda_{+,N}\psi) = (\psi_+, \tilde{W}\psi_+). \tag{A.2}$$

Noting that  $(\psi_+, T\psi_+) = (\psi_+, \sum_{k=1}^N D_0^{(k)}\psi_+) = (\psi, T_0\psi)$  and  $\|\Lambda_{+,N}\psi\| \leq \|\Lambda_{+,N}\|\|\psi\| \leq \|\psi\|$  because  $\|\Lambda_{+,N}\| = \|\Lambda_+^{(1)}\| \cdots \|\Lambda_+^{(n)}\| = 1$ , Lemma 7 is verified with the help of (A.1).

In order to show (A.1) we start by estimating from below. We use  $V^{(kl)} \geq 0$ ,  $|(\psi_+, V^{(k)}\psi_+)| \leq \frac{\gamma}{\gamma_{BR}} (\psi_+, E_{p_1}\psi_+)$  (for  $\gamma \leq \gamma_{BR}$ ; [4, 13]) as well as  $(\psi_+, B_{2m}^{(k)}\psi_+) \geq -md_0\gamma^2 (\psi_+, \psi_+)$  (for  $\gamma \leq 4/\pi$ ) with  $d_0 := 8 + 12\sqrt{2}$  [3, 13]. Then

$$(\psi_+, \tilde{W}\psi_+) \geq -\frac{\gamma}{\gamma_{BR}} \sum_{k=1}^N (\psi_+, E_{p_1}\psi_+) - md_0\gamma^2 \sum_{k=1}^N (\psi_+, \psi_+)$$

$$= -\frac{\gamma}{\gamma_{BR}} (\psi_+, T\psi_+) - md_0N\gamma^2 (\psi_+, \psi_+). \tag{A.3}$$

For the estimate from above we use  $(\psi_+, (V^{(k)} + B_{2m}^{(k)})\psi_+) \leq m(d_0\gamma^2 + \frac{3}{2}\gamma) (\psi_+, \psi_+)$  for  $\gamma \leq 4/\pi$  [3], [11, Lemma II.8] as well as  $(\psi_+, V^{(kl)}\psi_+) \leq \frac{e^2}{\gamma_{BR}} (\psi_+, E_{p_1}\psi_+)$  (for  $\gamma \leq \gamma_{BR}$ ) which is an immediate consequence of the estimate of  $V^{(k)}$ . Then

$$(\psi_+, \tilde{W}\psi_+) \leq m(d_0\gamma^2 + \frac{3}{2}\gamma)N (\psi_+, \psi_+) + \frac{N-1}{2} \frac{e^2}{\gamma_{BR}} (\psi_+, T\psi_+) \tag{A.4}$$

such that (A.1) holds with  $c_1 := \max\{\frac{\gamma}{\gamma_{BR}}, \frac{N-1}{2} \frac{e^2}{\gamma_{BR}}\}$ . For  $N \leq Z$ , one has  $c_1 = \frac{\gamma}{\gamma_{BR}}$  which is smaller than one if  $\gamma < \gamma_{BR}$ .

APPENDIX B (PROOF OF LEMMA 8)

For the proof of the relative boundedness of the total potential  $W_0$ , let  $H_N^{(2)} = T_0 + W_0 =: \Lambda_{+,N}(\sum_{k=1}^N D_0^{(k)} + W)\Lambda_{+,N}$  where  $W$  denotes the total potential from (3.1). Assume that

$$\|W\psi_+\| \leq c_0 \|\sum_{k=1}^N D_0^{(k)}\psi_+\| = c_0 \|T\psi_+\| \tag{B.1}$$

with  $\psi_+ = \Lambda_{+,N}\psi$ . Then

$$\begin{aligned} \|W_0\psi\| &= \|\Lambda_{+,N}W\Lambda_{+,N}\psi\| \leq \|\Lambda_{+,N}\| \|W\psi_+\| \leq c_0 \|\sum_{k=1}^N D_0^{(k)}\psi_+\| \\ &= c_0 \|\Lambda_{+,N} \sum_{k=1}^N D_0^{(k)}\Lambda_{+,N}\psi\| = c_0 \|T_0\psi\| \end{aligned} \tag{B.2}$$

since  $\Lambda_{+,N} = \Lambda_{+,N}^2$  commutes with  $D_0^{(k)}$ .

In order to verify (B.1) we set  $W^{(k)} := V^{(k)} + B_{2m}^{(k)}$  and estimate

$$\|W\psi_+\| \leq \|\sum_{k=1}^N W^{(k)}\psi_+\| + \|\sum_{k>l=1}^N V^{(kl)}\psi_+\| + 2\|\sum_{k>l=1}^N C_a^{(kl)}\psi_+\| + 2\|\sum_{k>l=1}^N C_b^{(kl)}\psi_+\| \tag{B.3}$$

where according to (2.2),  $C_a^{(kl)} := V^{(kl)}\Lambda_-^{(l)}F_0^{(l)}$  and  $C_b^{(kl)} := F_0^{(l)}\Lambda_-^{(l)}V^{(kl)} = C_a^{(kl)*}$ , and the antisymmetry of  $\psi_+$  with respect to particle exchange was used to reduce the four contributions to  $C^{(kl)}$  to two.

From [11] it follows that  $\|\sum_{k=1}^N W^{(k)}\psi_+\| \leq \sqrt{c_w} \|T\psi_+\|$  with  $c_w := (\frac{4}{3}\gamma + \frac{2}{9}\gamma^2)^2$  and  $\|V^{(kl)}\psi_+\| \leq \sqrt{c_v} \|E_{p_k}\psi_+\|$  with  $c_v := 4e^4$ . Likewise, using  $\|\Lambda_-^{(l)}\| = 1$

and  $\|F_0^{(l)}\| \leq \frac{\gamma}{\pi}(\frac{\pi^2}{4} - 1)$  [11], one has  $\|C_a^{(kl)}\psi_+\| \leq \sqrt{c_v} \|E_{p_k}(\Lambda_-^{(l)}F_0^{(l)}\psi_+)\| \leq \sqrt{c_v} \|F_0^{(l)}\| \|E_{p_k}\psi_+\| \leq \sqrt{\tilde{c}_s} \|E_{p_k}\psi_+\|$  and the same estimate for  $\|C_b^{(kl)}\psi_+\|$ , with  $\tilde{c}_s := (\frac{\gamma}{\pi}(\frac{\pi^2}{4} - 1))^2 c_v$  (for  $m = 0$ ). For the cross terms  $V^{(kl)}V^{(k'l')}$  ( $l \neq l'$ ) we substitute  $\mathbf{y}_l := \mathbf{x}_l - \mathbf{x}_k$  and  $\mathbf{y}_{l'} := \mathbf{x}_{l'} - \mathbf{x}_k$  for  $\mathbf{x}_l$  and  $\mathbf{x}_{l'}$ , respectively, and get

$$\begin{aligned}
 (\psi_+, V^{(kl)}V^{(k'l')}\psi_+) &= \int_{\mathbb{R}^{3N}} \left( \prod_{\substack{k'=1 \\ k' \neq l, l'}}^N d\mathbf{x}_{k'} \right) d\mathbf{y}_l d\mathbf{y}_{l'} \frac{e^2}{y_l} \bar{\psi}_+(\dots, \mathbf{y}_l + \mathbf{x}_k, \mathbf{y}_{l'} + \mathbf{x}_k, \dots) \\
 &\quad \cdot \frac{e^2}{y_{l'}} \psi_+(\dots, \mathbf{y}_l + \mathbf{x}_k, \mathbf{y}_{l'} + \mathbf{x}_k, \dots). \tag{B.4}
 \end{aligned}$$

Keeping for the moment  $\mathbf{x}_{k'}$  fixed and using the Fourier representation with respect to  $\mathbf{y}_l$  and  $\mathbf{y}_{l'}$  (setting  $\varphi_+(\mathbf{y}_l, \mathbf{y}_{l'}) := \psi_+(\dots, \mathbf{y}_l + \mathbf{x}_k, \mathbf{y}_{l'} + \mathbf{x}_k, \dots)$ ),

$$\widehat{\left(\frac{1}{y_l} \varphi_+\right)}(\mathbf{p}_l, \mathbf{p}_{l'}) = \frac{1}{2\pi^2} \int_{\mathbb{R}^3} d\mathbf{p}' \frac{1}{|\mathbf{p}_{l'} - \mathbf{p}'|^2} \hat{\varphi}_+(\mathbf{p}_l, \mathbf{p}'), \tag{B.5}$$

the Lieb and Yau formula (2.16) with the convergence generating function  $f(p) = p^{3/2}$  gives

$$\left| \int_{\mathbb{R}^6} d\mathbf{y}_l d\mathbf{y}_{l'} \frac{e^2}{y_l} \bar{\varphi}_+ \frac{e^2}{y_{l'}} \varphi_+ \right| \leq 4e^4 \int_{\mathbb{R}^6} d\mathbf{p}_l d\mathbf{p}_{l'} |\hat{\varphi}_+(\mathbf{p}_l, \mathbf{p}_{l'})|^2 p_l p_{l'} \tag{B.6}$$

such that, using  $p \leq E_p$ ,

$|(\psi_+, V^{(kl)}V^{(k'l')}\psi_+)| \leq c_v (\psi_+, p_l p_{l'} \psi_+) \leq c_v (\psi_+, E_{p_l} E_{p_{l'}} \psi_+)$ . The same estimate holds for  $V^{(kl)}V^{(k'l')}$  with distinct indices. The symmetry of  $\psi_+$  with respect to particle exchange and  $\sum_{k>l=1}^N 1 = \frac{N(N-1)}{2}$  then leads to the result

$$\left\| \sum_{k>l=1}^N V^{(kl)}\psi_+ \right\|^2 \leq c_v \cdot \max\left\{ \frac{N-1}{2}, \frac{1}{2} \left[ \frac{N(N-1)}{2} - 1 \right] \right\} \|T\psi_+\|^2.$$

The remaining contribution to (B.3) can partly be reduced to the estimate of  $V^{(kl)}$ . Let  $k, l, k', l'$  be distinct indices and set  $\varphi_l := \Lambda_-^{(l)}F_0^{(l)}\psi_+$ . Then we obtain

for the cross terms of  $(\sum_{k>l=1}^N C_a^{(kl)})^2$ ,

$$\begin{aligned}
 |(C_a^{(kl)}\psi_+, C_a^{(k'l')}\psi_+)| &= |(\Lambda_-^{(l)}F_0^{(l)}\psi_+, V^{(kl)}V^{(k'l')}\Lambda_-^{(l')}\psi_+)| \\
 &= |(\varphi_l, V^{(kl)}V^{(k'l')}\varphi_{l'})| \leq c_v (\varphi_l, p_k p_{k'} \varphi_l)^{\frac{1}{2}} (\varphi_{l'}, p_k p_{k'} \varphi_{l'})^{\frac{1}{2}}. \tag{B.7}
 \end{aligned}$$

Since  $l \neq k'$ ,  $p_{k'}$  commutes with  $\Lambda_-^{(l)}F_0^{(l)}$  such that

$$\begin{aligned}
 (\varphi_l, p_k p_{k'} \varphi_l) &= \|(p_k p_{k'})^{\frac{1}{2}} \varphi_l\|^2 = \|\Lambda_-^{(l)}F_0^{(l)}(p_k p_{k'})^{\frac{1}{2}} \varphi_l\|^2 \\
 &\leq \|F_0^{(l)}\|^2 (\psi_+, p_k p_{k'} \psi_+). \tag{B.8}
 \end{aligned}$$

The cross terms of  $(\sum_{k>l=1}^N C_b^{(kl)})^2$  have the same estimate. In fact,

$$\begin{aligned} |(C_b^{(kl)}\psi_+, C_b^{(k'l')}\psi_+)| &= |(\psi_+, V^{(kl)}\Lambda_-^{(l)}F_0^{(l)}F_0^{(l')}\Lambda_-^{(l')}V^{(k'l')}\psi_+)| \\ &= |(\varphi_{l'}, V^{(kl)}V^{(k'l')}\varphi_l)| \leq c_v \|F_0^{(l)}\|^2 (\psi_+, p_k p_{k'}\psi_+). \end{aligned} \tag{B.9}$$

If any two indices coincide, we use for simplicity a weaker estimate, e.g.

$$|(C_b^{(kl)}\psi_+, C_b^{(k'l')}\psi_+)| \leq \|C_b^{(kl)}\psi_+\| \|C_b^{(k'l')}\psi_+\| \leq \tilde{c}_s \|E_{p_k}\psi_+\|^2 \leq \tilde{c}_s \frac{1}{N} \|T\psi_+\|^2 \tag{B.10}$$

and similarly for  $C_a^{(kl)}$ .

Counting terms in the sum  $\sum_{k>l=1}^N C_a^{(kl)} \sum_{k'>l'=1}^N C_a^{(k'l')}$  we have  $\frac{N(N-1)}{2}$  square terms,  $\frac{1}{4}N(N-1)(N-2)(N-3)$  terms with four distinct indices and  $N(N-1)(N-2)$  terms where two of the four indices agree (while the other two are distinct). For all terms of the last type, the estimate (B.10) is used whereas for the other terms we proceed as in the case of  $(\sum_{k>l=1}^N V^{(kl)})^2$ . This leads to

$$\begin{aligned} \left\| \sum_{k>l=1}^N C_a^{(kl)}\psi_+ \right\|^2 &\leq \tilde{c}_s \cdot \max\left\{ \frac{N-1}{2}, \frac{(N-2)(N-3)}{4} \right\} \|T\psi_+\|^2 \\ &\quad + \tilde{c}_s (N-1)(N-2) \|T\psi_+\|^2. \end{aligned} \tag{B.11}$$

Inserting our results into (B.3) we find  $\|W\psi_+\| \leq c_0 \|T\psi_+\|$  with

$$\begin{aligned} c_0 &:= \sqrt{c_w} + \sqrt{c_v \cdot \max\left\{ \frac{N-1}{2}, \frac{1}{2} \left[ \frac{N(N-1)}{2} - 1 \right] \right\}} \\ &\quad + 4 \sqrt{\tilde{c}_s} \sqrt{\max\left\{ \frac{N-1}{2}, \frac{(N-2)(N-3)}{4} \right\} + (N-1)(N-2)}. \end{aligned} \tag{B.12}$$

For  $N = Z$  we get  $c_0 < 1$  for  $\gamma < 0.285$  which corresponds to  $Z \leq 39$ . For  $N = 2$ , we need  $\gamma < 0.66$  ( $Z \leq 90$ ) which slightly improves on our earlier estimate ( $Z \leq 89$  [11]), obtained by using (B.10)-type estimates for all two-particle interaction cross terms.

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