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EXISTENCE OF A MINIMIZER FOR THE QUASI-RELATIVISTIC KOHN-SHAM MODEL

C. ARGAEZ AND M. MELGAARD

Abstract. We study the standard and extended Kohn-Sham models for quasi-relativistic N-electron Coulomb systems; that is, systems where the kinetic energy of the electrons is given by the quasi-relativistic operator

$$\sqrt{-\alpha^{-2}\Delta_{x_n}+\alpha^{-4}}-\alpha^{-2}.$$

For spin-unpolarized systems in the local density approximation, we prove existence of a ground state (or minimizer) provided that the total charge $Z_{\rm tot}$ of K nuclei is greater than $N-1$ and that $Z_{\rm tot}$ is smaller than a critical charge $Z_{\rm c}=2\alpha^{-1}\pi^{-1}$.

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1. Introduction

The Density Functional Theory (DFT) of Kohn and Sham has emerged as the most widely-used method of electronic structure calculation in both quantum chemistry and condensed matter physics [11, 18]. In this paper we establish existence of a ground state (or minimizer) for the quasi-relativistic spin-unpolarized (or restricted) Kohn-Sham problem given by

$$I_N^{\mathrm{RKS}}(V) = \inf\Big\{\mathcal{E}(\mathbf{\Phi}) := \alpha^{-1}\sum_{n=1}^{N_{\mathrm{p}}}\int_{\mathbb{R}^3}\Big(|T_0^{1/2}\phi_n|^2 - |\phi_n|^2\Big) + \int_{\mathbb{R}^3} V\rho_{\mathbf{\Phi}} + \mathcal{J}(\rho_{\mathbf{\Phi}}) + E_{\mathrm{xc}}(\rho_{\mathbf{\Phi}}),\ \rho_{\mathbf{\Phi}} = 2\sum_{n=1}^{N_{\mathrm{p}}}|\phi_n|^2,\ \mathbf{\Phi}\in\mathcal{C}_{N_{\mathrm{p}}}\Big\} \tag{1.1}$$

with

$$\mathcal{C}_{N_{\mathrm{p}}} = \{\mathbf{\Phi} = (\phi_1,\dots,\phi_{N_{\mathrm{p}}}) \in \mathbf{H}^{1/2}(\mathbb{R}^3)^{N_{\mathrm{p}}} : \langle\phi_m,\phi_n\rangle_{L^2(\mathbb{R}^3)} = \delta_{mn}\} \tag{1.2}$$

Here $T_0 = \sqrt{-\Delta_{x_n} + \alpha^{-2}}$ is (essentially) the quasi-relativistic kinetic energy of the nth electron located at $x_n \in \mathbb{R}^3$ (Δ_{x_n} being the Laplacian with respect to x_n), α is Sommerfeld's fine structure constant, $\mathbf{H}^{1/2}(\mathbb{R}^3)$ is the Sobolev space in (2.1), $V(\cdot)$ is the attractive interaction between an electron and the K nuclei (with changes $Z_k > 0$, $k = 1, 2, \dots, K$)

$$V_{\mathrm{en}}(\mathbf{r}) = \sum_{k=1}^{K} V_k(\mathbf{r}); \quad V_k(\mathbf{r}) = -\frac{Z_k\alpha}{|\mathbf{r}-\mathbf{R}_k|}, \tag{1.3}$$

the Coulomb energy $\mathcal{J}(\cdot)$ is given by

$$\mathcal{J}(\rho) = \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}d\mathbf{r}', \tag{1.4}$$

where the density is

$$\rho_{\mathbf{\Phi}}(\mathbf{r}) = \sum_{n=1}^{N}\sum_{\sigma\in\Sigma}|\phi_n(\mathbf{r},\sigma)|^2. \tag{1.5}$$

We limit ourselves to systems with an even number of electrons $N = 2N_{\mathrm{p}}$, where N_{p} is the number of electron pairs. The exchange-correlation functional is chosen as

$$E_{\mathrm{xc}}(\rho) = \int_{\mathbb{R}^3} g\left(\rho(\mathbf{r})\right)\, d\mathbf{r}, \tag{1.6}$$

yielding the local density approximation (abbreviated LDA), and the following assumptions imposed on the function g ensure that (1.6) incorporates all approximate LDA functionals used in practical implementations (see, e.g., [19]).

Assumption 1.1. Let g be a twice differentiable function which satisfies

$$g \in C^1(\mathbb{R}_+, \mathbb{R}) \tag{1.7}$$

$$g(0) = 0 \tag{1.8}$$

$$g' \leq 0 \tag{1.9}$$

$$\exists\, 0 < \beta_- \leq \beta_+ < 1/3 \text{ such that } \sup_{\rho \in \mathbb{R}_+} \frac{|g'(\rho)|}{\rho^{\beta_-} + \rho^{\beta_+}} < \infty \tag{1.10}$$

$$\exists\, 1 \leq \gamma < 3/2 \text{ such that } \limsup_{\rho \to 0^+} \frac{g(\rho)}{\rho^\gamma} < 0 \tag{1.11}$$

We establish the following theorem for the minimization problem (1.1)-(1.2) and its extended version formulated in (4.2)-(4.3).

Theorem 1.2. *Suppose that $N = 2N_{\mathrm{p}} \leq Z_{\mathrm{tot}} < Z_{\mathrm{c}} = 2\alpha^{-1}\pi^{-1}$ and let Assumption 1.1 be satisfied. Then the extended Kohn-Sham LDA problem* (4.2)-(4.3) *has a minimizer $\mathcal{D}$ satisfying*

$$\mathcal{D} = \chi_{(-\infty, \epsilon_F)}\left(T_{\rho_\mathcal{D}}\right) + \mathcal{D}^{(\delta)} \tag{1.12}$$

for some ϵ_F, where

$$T_{\rho_\mathcal{D}} = \alpha^{-1}\widetilde{T}_0 + \alpha^{-1}V + \rho_\mathcal{D} * \frac{1}{|\mathbf{r}|} + g'(\rho_\mathcal{D}), \tag{1.13}$$

with $\chi_{(-\infty,\epsilon_F)}$ being the characteristic function of the range $(-\infty, \epsilon_F)$ and with $\mathcal{D}^{(\delta)} \in \mathcal{S}(L^2(\mathbb{R}^3))$ satisfying $0 \leq \mathcal{D}^{(\delta)} \leq 1$ and $\mathrm{Ran}(\mathcal{D}^{(\delta)}) \subset \mathrm{Ker}(T_{\rho_\mathcal{D}} - \epsilon_F)$. (We refer to Section 4 for the definition of $\widetilde{T}_0$ and $\mathcal{S}(L^2(\mathbb{R}^3))$).

Few rigorous results on Kohn-Sham theory are found in the mathematical literature. In the non-relativistic setting, Le Bris [12, 13] treated the standard Kohn-Sham model. Le Bris proved existence of a ground state using concentration-compactness type arguments as pioneered by Lions in his work on Thomas-Fermi type models [15, 16]. Our result, covering both the standard and extended Kohn-Sham models, is the analogue of the recent non-relativistic result by Anantharaman and Cancès [2, Theorem 1] and we follow the same scheme of proof. In addition to the usual mathematical difficulties for these models (nonlinearity, nonconvexity and the possible loss of compactness at infinity), the quasi-relativistic setting requires that almost all arguments have to be addressed anew because the underlying single-particle Hilbert space is $\mathbf{H}^{1/2}(\mathbb{R}^3)$ instead of $\mathbf{H}^1(\mathbb{R}^3)$ and, furthermore, the kinetic energy is described by a nonlocal, pseudodifferential operator. Moreover, the Coulomb potential is not relatively compact (in the operator sense) with respect to the quasi-relativistic energy operator. In particular, the energy functional is not weakly lower semicontinuous in the usual sense. Nevertheless, one can establish a decreasing property, see Section 6, which suffices for our purpose.

The quasi-relativistic setting has attracted substantial interest lately. Enstedt and Melgaard [8] established existence of infinitely many distinct solutions to the quasi-relativistic Hartree-Fock equations, including a ground state. The results are valid under the hypotheses that the total charge Z_{tot} of K nuclei is greater than $N-1$ and that Z_{tot} is smaller than the above-mentioned critical charge Z_{c}. The proofs are based on a new application of the Lions-Fang-Ghoussoub critical point approach to multiple solutions on a complete, C^2 Hilbert-Riemann manifold. Existence of a ground state for an atom was first addressed by Dall'Acqua et al [5], who applied the relaxation method by Lieb and Simon. In addition, regularity of the ground state away from the nucleus and pointwise exponential decay of the orbitals were established in [5]. Furthermore, Dall'Acqua and Solovej [6] have shown that the maximal negative ionization charge and the ionization energy of an atom remain bounded independently of the nuclear charge and the fine structure constant provided their product is bounded. In a recent work, Argaez and Melgaard [3] have proved existence of infinitely many solutions, finitely many being interpreted as excited states, to the multi-configurative quasi-relativistic Hartree-Fock type equations. Furthermore, Melgaard and Zongo have shown existence of multiple solutions to the Choquard equation in the quasi-relativistic setting [17].

2. Preliminaries

Throughout this article, we denote by c and C (with or without indices) various positive constants whose precise value is of no importance. Moreover, we will denote the complex conjugate of $z \in \mathbb{C}$ by $\overline{z}$.

Function spaces. For $1 \leq p \leq \infty$, let $L^p(\mathbb{R}^3)$ be the space of (equivalence classes of) complex-valued functions ϕ which are measurable and satisfy $\int_{\mathbb{R}^3} |\phi(x)|^p \,\mathrm{d}x < \infty$ if $p < \infty$ and $\|\phi\|_{L^\infty(\mathbb{R}^3)} = \operatorname{ess\,sup} |\phi| < \infty$ if $p = \infty$. The measure $\mathrm{d}x$ is the Lebesgue measure. For any p the $L^p(\mathbb{R}^3)$ space is a Banach space with norm $\|\cdot\|_{L^p(\mathbb{R}^3)} = (\int_{\mathbb{R}^3} |\cdot|^p \,\mathrm{d}x)^{1/p}$. In the case $p = 2$, $L^2(\mathbb{R}^3)$ is a complex and separable Hilbert space with scalar product $\langle \phi, \psi \rangle_{L^2(\mathbb{R}^3)} = \int_{\mathbb{R}^3} \phi\overline{\psi}\mathrm{d}x$ and corresponding norm $\|\phi\|_{L^2(\mathbb{R}^3)} = \langle \phi, \phi \rangle_{L^2(\mathbb{R}^3)}^{1/2}$. Similarly, $L^2(\mathbb{R}^3)^N$, the N-fold Cartesian product of $L^2(\mathbb{R}^3)$, is equipped with the scalar product $\langle \phi, \psi \rangle = \sum_{n=1}^N \langle \phi_n, \psi_n \rangle_{L^2(\mathbb{R}^3)}$. The space of infinitely differentiable complex-valued functions with compact support will be denoted $C_0^\infty(\mathbb{R}^3)$. The Fourier transform is given by

$$(\mathcal{F}\,\psi)(\xi) = \hat{\psi}(\xi) = (2\pi)^{-1/2} \int_{\mathbb{R}^3} e^{-ix\xi} \psi(x) \,\mathrm{d}x.$$

Define

$$\mathbf{H}^{1/2}(\mathbb{R}^3) = \{\phi \in L^2(\mathbb{R}^3) : (1+|\xi|)^{1/2}\hat{\phi} \in L^2(\mathbb{R}^3)\}, \tag{2.1}$$

which, equipped with the scalar product

$$\langle \phi, \psi \rangle_{\mathbf{H}^{1/2}(\mathbb{R}^2)} = \int_{\mathbb{R}^3} (1+|\xi|)\hat{\phi}(\xi)\overline{\hat{\psi}(\xi)}\, d\xi,$$

becomes a Hilbert space; evidently, $\mathbf{H}^1(\mathbb{R}^3) \subset \mathbf{H}^{1/2}(\mathbb{R}^3)$. We have that $C_0^\infty(\mathbb{R}^3)$ is dense in $\mathbf{H}^{1/2}(\mathbb{R}^3)$ and the continuous embedding $\mathbf{H}^{1/2}(\mathbb{R}^3) \hookrightarrow L^r(\mathbb{R}^3)$ holds whenever $2 \le r \le 3$ [1].

Moreover, we shall use that any weakly convergent sequence in $\mathbf{H}^{1/2}(\mathbb{R}^3)$ converges strongly in $L^p_{\mathrm{loc}}(\mathbb{R}^3)$, $p < 3$, and it has a pointwise convergent subsequence. Standard arguments yield the following result; an analogue of Lions' result [15, Part II, Lemma I.1].

Proposition 2.1. *Let $r > 0$ and $2 \le q < 3$. If the sequence $\{u_j\}$ is bounded in $\mathbf{H}^{1/2}(\mathbb{R}^3)$ and if*

$$\sup_{y\in\mathbb{R}^3} \int_{B(y,r)} |u_j|^q \to 0 \quad \text{as } j \to \infty$$

then $u_j \to 0$ in $L^r(\mathbb{R}^3)$ for any $2 < r < 3$.

Operators. Let T be a self-adjoint operator on a Hilbert space $\mathcal{H}$ with domain $\mathfrak{D}(T)$. The spectrum and resolvent set are denoted by $\mathrm{spec}(T)$ and $\rho(T)$, respectively. We use standard terminology for the various parts of the spectrum; see, e.g., [7, 10]. The resolvent is $R(\zeta) = (T-\zeta)^{-1}$. The spectral family associated to T is denoted by $E_T(\lambda)$, $\lambda \in \mathbb{R}$. For a lower semi-bounded self-adjoint operator T, the counting function is defined by

$$\mathrm{Coun}(\lambda; T) = \dim \mathrm{Ran}\, E_T((-\infty, \lambda)).$$

The space of trace operators, respectively, Hilbert-Schmidt operators, on $\mathfrak{h} = L^2(\mathbb{R}^3)$ is denoted by $\mathfrak{S}_1(\mathfrak{h})$, respectively $\mathfrak{S}_2(\mathfrak{h})$ or, in short, $\mathfrak{S}_j$, $j = 1, 2$. The space of bounded self-adjoint operators is designated by $\mathcal{S}(\mathfrak{h})$.

We need the following abstract operator result by Lions [16, Lemma II.2].

Lemma 2.2. *Let T be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and let $\mathcal{H}_1$, $\mathcal{H}_2$ be two subspaces of $\mathcal{H}$ such that $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$, $\dim \mathcal{H}_1 = \mathsf{h}_1 < \infty$ and $P_2TP_2 \ge 0$, where P_2 is the orthogonal projection onto $\mathcal{H}_2$. Then T has at most h_1 negative eigenvalues.*

3. Atomic and molecular Hamiltonians

By p we denote the momentum operator $-i\nabla$ on $L^3(\mathbb{R}^3)$. The operator $T_0 = \sqrt{p^2 + \alpha^{-2}}$ is generated by the closed, (strictly) positive form

$$\mathfrak{t}_0[\phi, \phi] = \langle T_0^{1/2}\phi, T_0^{1/2}\phi \rangle_{\mathcal{H}}$$

on the form domain $\mathfrak{D}(\mathfrak{t}_0) = \mathbf{H}^{1/2}(\mathbb{R}^3)$. Set $S(x) = Z\alpha/|x|$, $Z > 0$, $Z_{\rm c} = 2\alpha^{-1}\pi^{-1}$, and let $\widetilde{T}_0 = T_0 - \alpha^{-1}$. The following facts are well-known for the perturbed one-particle operator $H_{1,1,\alpha} = \widetilde{T}_0 - S(x)$ [9, 10].

Small perturbations. If $Z < \frac{\pi}{2} Z_{\rm c}$ then S is $\widetilde{T}_0$-bounded with relative bound equal to two. If, on the other hand, $(2\alpha)^{-1} < Z < Z_{\rm c}$ then S is $\widetilde{T}_0$-form bounded with relative bound less than one.

We prove the above-mentioned form-boundedness. It follows from the following inequality (first observed, it seems, by Kato [10, Paragraph V-§5.4]):

$$\langle S\phi, \phi\rangle_{L^2(\mathbb{R}^3)} \leq (Z/Z_{\rm c})\|\phi\|^2_{\mathbf{H}^{1/2}(\mathbb{R}^3)}, \quad \forall \phi \in \mathbf{H}^{1/2}(\mathbb{R}^3). \tag{3.1}$$

Indeed, if, for any $\psi, \phi \in \mathbf{H}^{1/2}(\mathbb{R}^3)$, we define the sesquilinear forms

$$\begin{aligned} \mathfrak{s}[\psi, \phi] &:= \langle S^{1/2}\psi, S^{1/2}\phi\rangle_{L^2(\mathbb{R}^3)}, \\ \mathfrak{t}_0[\psi, \phi] &:= \langle T_0^{1/2}\psi, T_0^{1/2}\phi\rangle_{L^2(\mathbb{R}^3)}, \\ \tilde{\mathfrak{t}}_0[\psi, \phi] &:= \mathfrak{t}_0[\psi, \phi] - \alpha^{-1}\langle \psi, \phi\rangle_{L^2(\mathbb{R}^3)}, \end{aligned}$$

then (3.1) shows that $\mathfrak{s}$ is well-defined and also, by invoking the inequality $|-i\nabla| \leq T_0$, we infer that, for all $\phi \in \mathbf{H}^{1/2}(\mathbb{R}^3)$,

$$\mathfrak{s}[\phi, \phi] < \mathfrak{t}_0[\phi, \phi] \quad \text{provided } Z < Z_{\rm c}. \tag{3.2}$$

This is the *Coulomb uncertainty principle* in the quasi-relativistic setting. The KLMN theorem (see, e.g., [10, Paragraph VI-1.7]) implies that there exists a unique self-adjoint operator, denoted $H_{1,1,\alpha}$, generated by the closed sesquilinear form

$$\mathfrak{h}_{1,1,\alpha}[\psi, \phi] := \tilde{\mathfrak{t}}_0[\psi, \phi] - \mathfrak{s}[\psi, \phi], \quad \psi, \phi \in \mathfrak{D}(\mathfrak{h}_{1,1,\alpha}) = \mathbf{H}^{1/2}(\mathbb{R}^3), \tag{3.3}$$

which is bounded below by $-\alpha^{-1}$. It is well-known [9] that

$$\begin{aligned} \operatorname{spec}(H_{1,1,\alpha}) \cap [-\alpha^{-1}, 0) &\quad \text{is discrete} \\ \operatorname{spec}(H_{1,1,\alpha}) \cap [0, \infty) &\quad \text{is absolutely continuous} \end{aligned} \tag{3.4}$$

In particular,

$$\operatorname{spec}_{\rm ess}(H_{1,1,\alpha}) = [0, \infty). \tag{3.5}$$

The form construction of the atomic Hamiltonian $H_{1,1,\alpha}$ can be generalized to the molecular case, describing a molecule with N electrons and K nuclei of charges $\mathbf{Z} = (Z_1, \ldots, Z_K)$, $Z_k > 0$, located at $R_1, \ldots, R_K$, $R_k \in \mathbb{R}^3$, if we substitute $\mathfrak{s}$ by

$$\mathfrak{v}_{\rm en}[\psi, \phi] = \sum_{k=1}^{K} \langle V_k^{1/2}, \psi, V_k^{1/2}\phi\rangle, \quad \psi, \phi \in \mathbf{H}^{1/2}(\mathbb{R}^3), \tag{3.6}$$

where V_k is defined in (1.3) and by assuming that $Z_{\rm tot} < Z_{\rm c}$.

We shall use the following IMS-type localization estimate [14, Lemma A.1].

Lemma 3.1. *Suppose* $\{\xi_j\}_{j\in J}$ *is a smooth partition of unity such that* $\sum_{j\in J}\xi_j(x)^2$
$\equiv 1$ *and* $\nabla\xi_j \in L^s(\mathbb{R}^n)$ *with* $s \in (2n, \infty]$*. Then the following IMS type estimate holds for* T_0*:*

$$T_0 \geq \sum_{j\in J} \xi_j T_0 \xi_j - \frac{1}{\pi}\int_0^\infty \frac{1}{T_0^2+\tau}\Big(\sum_{j\in J} |\nabla\xi_j|^2\Big)\frac{1}{T_0^2+\tau}\sqrt{\tau}\,d\tau.$$

Moreover, we need the following spectral result found in [8]. Its proof is based on Glazman's lemma for the counting function (see, e.g, [20, Lemma A.3]).

Lemma 3.2. *Assume* $\vartheta < Z_{\mathrm{tot}} < Z_{\mathrm{c}}$*, and let* $\rho \in L^1(\mathbb{R}^3) \cap L^{4/3}(\mathbb{R}^3)$ *such that* $\int_{\mathbb{R}^3}\rho\,\mathrm{d}x < \vartheta$*. Define the quasi-relativistic Schrödinger operator*

$$T = \alpha^{-1}\widetilde{T}_0 + \alpha^{-1}V_{\mathrm{en}} + \rho * \frac{1}{|x|}.$$

Then, for any $\kappa \geq 1$ *and any* $0 \leq \vartheta < Z_{\mathrm{tot}}$*, there exists* $\epsilon_{\kappa,\vartheta} > 0$ *such that* $\mathrm{Coun}(-\epsilon_{n,\vartheta}; T) \geq \kappa$*.*

4. Density operator framework

To turn the minimization problem (1.1)-(1.2) into a convex problem, we proceed to extend the definition of the restricted Kohn-Sham (RKS) energy functional. We can re-express the RKS functional and the Kohn-Sham ground state energy via the one-to-one correpondence between elements of $\mathcal{C}_{N_{\mathrm{p}}}$ and projections onto finite-dimensional subspaces of $L^2(\mathbb{R}^3)$. Indeed, given an element $\{\phi_n\}_{n=1}^N$ in $\mathcal{C}_{N_{\mathrm{p}}}$ we can associate a canonical projection operator, $\mathcal{D} = \sum_{n=1}^N \langle\cdot,\phi_n\rangle\phi_n$ with trace equal to N. We may therefore write the RKS energy functional as

$$\mathcal{E}(\mathcal{D}) = \alpha^{-1}\left(\mathrm{Tr}\left[\widetilde{T}_0\mathcal{D}\right] - \mathrm{Tr}[V_{\mathrm{en}}\mathcal{D}]\right) + \mathcal{J}(\rho_{\mathcal{D}}) + E_{\mathrm{xc}}(\rho_{\mathcal{D}}), \tag{4.1}$$

where

$$\mathrm{Tr}[\widetilde{T}_0\mathcal{D}] = \sum_{n=1}^N \mathfrak{t}_0[\phi_n,\phi_n] - \alpha^{-1}[\phi_n,\phi_n]$$

$$\mathrm{Tr}[V_{\mathrm{en}}\mathcal{D}] = \sum_{n=1}^N \mathfrak{v}_{\mathrm{en}}[\phi_n,\phi_n]$$

The *direct Coulomb energy* defined (in terms of the Coulomb inner product) as

$$\mathcal{J}(\rho_{\mathcal{D}}) = \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\rho_{\mathcal{D}}(\mathbf{r})|\mathbf{r}-\mathbf{r}'|^{-1}\rho_{\mathcal{D}}(\mathbf{r}')\,d\mathbf{r}\,d\mathbf{r}'$$

and the exchange-correlation functional defined as in (1.6). Then we embed (1.1)-(1.2) in the collection of problems

$$I_\lambda = \inf\{\mathcal{E}(\mathcal{D}) : \mathcal{D} \in \mathcal{K}_\lambda\} \tag{4.2}$$

parametrized by $\lambda \in \mathbb{R}_+$, where

$$\mathcal{K}_\lambda = \{\mathcal{D} \in \mathcal{S}(L^2(\mathbb{R}^3)) : 0 \le \mathcal{D} \le 1,\ \mathrm{Tr}(\mathcal{D}) = \lambda,\ \mathrm{Tr}(T_0\mathcal{D}) < \infty\}, \tag{4.3}$$

with $\mathcal{S}(L^2(\mathbb{R}^3))$ being the space of all bounded, self-adjoint operators on $L^2(\mathbb{R}^3)$. Likewise, we introduce the problem at infinity

$$I_\lambda^\infty = \inf\{\mathcal{E}^\infty(\mathcal{D}) : \mathcal{D} \in \mathcal{K}_\lambda\}, \tag{4.4}$$

where

$$\mathcal{E}^\infty(\mathcal{D}) = \alpha^{-1}\,\mathrm{Tr}(\widetilde{T}_0\mathcal{D}) + \mathcal{J}(\rho_{\mathcal{D}}) + E_{\mathrm{xc}}(\rho_{\mathcal{D}}). \tag{4.5}$$

The operator $\mathcal{D}$ is the so-called (reduced) one-particle density operator. The general theory of trace class operators on $L^2(\mathbb{R}^3)$ asserts that any operator $\mathcal{D}$ in $\mathcal{K}$ admits a complete set of eigenfunctions $\{\phi_i\}$ in $\mathbf{H}^{1/2}(\mathbb{R}^3)$ associated to the eigenvalues $\nu_n \in [0,1]$, counted with multiplicity. Hence we may decompose $\mathcal{D}$ along such an eigenbasis of $L^2(\mathbb{R}^3)$, in such a way that its Hilbert-Schmidt kernel may be written as

$$\rho(x,y) = \sum_{n\ge1} \nu_n \phi_n(x)\overline{\phi_n(y)}.$$

Since $\mathcal{D}$ is trace class, the corresponding density is well-defined as a nonnegative function in $L^1(\mathbb{R}^3)$ through $\rho(x,x) = \sum_{n\ge1}\nu_n|\phi_n(x)|^2$, and $\mathrm{Tr}\,\mathcal{D} = \int_{\mathbb{R}^3}\rho(x,x)\,dx = \sum_{n\ge1}\nu_n$. Furthermore, the spectral decomposition of $\mathcal{D}$ enable us to give sense to

$$\mathrm{Tr}[T_0\mathcal{D}] = \sum_{n\ge1}\nu_n\int_{\mathbb{R}^3}|T_0^{1/2}\phi_n(x)|^2\,dx. \tag{4.6}$$

We introduce the vector space

$$\mathcal{H} = \left\{\mathcal{D} \in \mathfrak{S}_1 : T_0^{1/2}\mathcal{D}T_0^{1/2} \in \mathfrak{S}_1\right\}$$

equipped with the norm $\|\cdot\|_{\mathcal{H}} = \mathrm{Tr}(\cdot) + \mathrm{Tr}(T_0^{1/2}\cdot T_0^{1/2})$. Furthermore, we introduce the convex set

$$\mathcal{K} = \{\mathcal{D} \in \mathcal{S}(\mathfrak{h}) : 0 \le \mathcal{D} \le 1, \quad \mathrm{Tr}(\mathcal{D}) < \infty, \quad \mathrm{Tr}(T_0^{1/2}\mathcal{D}T_0^{1/2}) < \infty\}.$$

5. Concentration-compactness type inequalities

The aim of this section is to establish concentration-compactness type inequalities, see Proposition 5.5. To achieve this we need to prove a series of auxiliary results.

Lemma 5.1. *For any $\mathcal{D} \in \mathcal{K}$ one has $\sqrt{\rho_{\mathcal{D}}} \in \mathbf{H}^{1/2}(\mathbb{R}^3)$ and, moreover, the following inequalities are valid:*
Lower bound on the kinetic energy:

$$\|\sqrt{\rho_{\mathcal{D}}}\|^2_{\mathbf{H}^{1/2}(\mathbb{R}^3)} \le C \operatorname{Tr}[T_0\mathcal{D}], \tag{5.1}$$

$$\operatorname{Tr}[\mathcal{D}] \le C \operatorname{Tr}[T_0\mathcal{D}] \tag{5.2}$$

Upper bound on Coulomb energy:

$$0 \le \mathcal{J}(\rho_{\mathcal{D}}) \le C \operatorname{Tr}[T_0\mathcal{D}] \operatorname{Tr}[\mathcal{D}] \tag{5.3}$$

Bounds on nuclei-electron interaction: For $Z_{\mathrm{tot}} < Z_{\mathrm{c}} = 2/(\alpha\pi)$,

$$-C \operatorname{Tr}[T_0\mathcal{D}] \le \int V_{\mathrm{en}}\rho_{\mathcal{D}}\, dx \le 0. \tag{5.4}$$

Bounds on exchange correlation energy:

$$\begin{aligned} &- C \left(\operatorname{Tr}[\mathcal{D}]^{1-\frac{\beta_-}{2}} (\operatorname{Tr}[T_0\mathcal{D}])^{3\beta_-} + \operatorname{Tr}[\mathcal{D}]^{1-\frac{\beta_+}{2}} (\operatorname{Tr}[T_0\mathcal{D}])^{3\beta_+} \right) \\ &\le E_{xc}(\rho_{\mathcal{D}}) \le 0. \end{aligned} \tag{5.5}$$

Proof. We shall prove the inequalities in the order of appearance. Inequality (5.1): For any

$$\mathcal{D} = \sum \nu_n \,|\phi_n\rangle\langle\phi_n|\,, \quad \nu_n \in [0,1],$$

we have

$$\operatorname{Tr}(T_0\mathcal{D}) = \sum \nu_n \langle T_0^{1/2}\phi_n, T_0^{1/2}\phi_n\rangle\,.$$

From the convexity of the relativistic kinetic energy; i.e., for any $\phi, \psi \in \mathbf{H}^{1/2}(\mathbb{R}^3)$,

$$\langle \sqrt{|\phi|^2 + |\psi|^2}, \widetilde{T}_0\sqrt{|\phi|^2 + |\psi|^2}\rangle \le \langle \phi, \widetilde{T}_0\phi\rangle + \langle \psi, \widetilde{T}_0\psi\rangle$$

we obtain

$$\begin{aligned} \langle \sqrt{\rho_{\mathcal{D}}}, \widetilde{T}_0\sqrt{\rho_{\mathcal{D}}}\rangle &= \Big\langle \Big(\sum_n \nu_n|\phi_n|^2\Big)^{1/2}, \widetilde{T}_0\Big(\sum_n \nu_n|\phi_n|^2\Big)^{1/2}\Big\rangle \\ &\le \sum_n \nu_n\langle \phi_n, \widetilde{T}_0\phi_n\rangle = \operatorname{Tr}[\widetilde{T}_0\mathcal{D}]. \end{aligned}$$

Inequality (5.2) follows from (5.1) and the Sobolev inequality for $\mathbf{H}^{1/2}(\mathbb{R}^3)$.

Inequality (5.3): We apply the Hardy-Littlewood-Sobolev inequality, L^p interpolation, and the inequality (5.2) to get

$$\begin{aligned} \mathcal{J}(\rho_{\mathcal{D}}) \le C_1\|\rho_{\mathcal{D}}\|_{L^{6/5}} &\le C_1\|\rho_{\mathcal{D}}\|_{L^{3/2}}\|\rho_{\mathcal{D}}\|_{L^1} \\ &\le C_2 \operatorname{Tr}[\mathcal{D}] \operatorname{Tr}[T_0\mathcal{D}]. \end{aligned}$$

Inequality (5.4): The Hardy-Kato inequality (3.1), together with (5.1), yields

$$\int_{\mathbb{R}^3} \frac{\rho_{\mathcal{D}}}{|\mathbf{r} - \mathbf{R}_k|}\, d\mathbf{r} \le C_1 \sum_n \|\phi_n\|^2_{\mathbf{H}^{1/2}} \le C_2 \operatorname{Tr}(T_0\mathcal{D})$$

whence (5.4) follows.

Inequality (5.5): We see from Assumption 1.1 that $E_{\mathrm{xc}}(\rho) \leq 0$. From the fundamental theorem of calculus and (1.7)-(1.10) we have that

$$|g(\rho)| = \Big| \int_0^\rho g'(\tilde{\rho})\, d\tilde{\rho}\Big| \leq C_2\big(\rho^{1+\beta_-} + \rho^{1+\beta_+}\big)$$

and, therefore, with $p_\pm = 1 + \beta_\pm$,

$$|E_{\mathrm{xc}}(\rho)| = \Big| \int_{\mathbb{R}^3} g(\rho(\mathbf{r}))\, d\mathbf{r}\Big| \leq C\Big(\int_{\mathbb{R}^3} \rho^{p_-}\, d\mathbf{r} + \int_{\mathbb{R}^3} \rho^{p_+}\, d\mathbf{r}\Big). \tag{5.6}$$

Now, using L^p interpolation and (5.2), we obtain

$$\int_{\mathbb{R}^3} \rho^{1+\beta_\pm}\, d\mathbf{r} = \|\rho\|_{L^{1+\beta_\pm}}^{1+\beta_\pm} \leq \|\rho\|_{L^1}^{1-2\beta_\pm} \|\rho\|_{L^{3/2}}^{3\beta_\pm} \leq C(\mathrm{Tr}[\mathcal{D}])^{1-2\beta_\pm}(\mathrm{Tr}[T_0\mathcal{D}])^{3\beta_\pm}$$

From this we immediately get (5.5). □

Lemma 5.2. *The functionals $\mathcal{E}$ and $\mathcal{E}^\infty$ are continuous on $\mathcal{H}$.*

Proof. By definition of the norm in $\mathcal{H}$, $\mathcal{D} \mapsto \mathrm{Tr}(\widetilde{T_0}\mathcal{D})$ is continuous on $\mathcal{H}$. For the term $\int V u^2$, the continuity follows from the Cauchy-Schwarz inequality and the Hardy-Kato inequality (3.1):

$$\begin{aligned} \Big| \int V u^2 - V\tilde{u}^2 \Big| &\leq \int V|u - \tilde{u}||u + \tilde{u}|\, dx \\ &\leq C \int V|u - \tilde{u}|^2 \leq C\|u - \tilde{u}\|_{\mathbf{H}^{1/2}}^2 \end{aligned}$$

Let $W := 1/|x| = W_1 + W_2$ where $W_1 \in L^4$ and $W \in L^\infty$. For the term $J(\cdot)$ the estimate

$$\begin{aligned} |J(\rho) - J(\tilde{\rho})| &= \Big|\frac{1}{2}\int [(\rho - \tilde{\rho}) * W](\rho + \tilde{\rho})\, dx\Big| \\ &\leq C\|\rho - \tilde{\rho}\|_{L^1}\left(\|W_1\|_{L^4}\|\rho - \tilde{\rho}\|_{L^{4/3}} + \|W_2\|_{L^\infty}\|\rho + \tilde{\rho}\|_{L^1}\right) \end{aligned}$$

establishes the continuity. Now,

$$\begin{aligned} |E_{\mathrm{xc}}(\rho_{\mathcal{D}_j}) - E_{\mathrm{xc}}(\rho_{\mathcal{D}})| &\leq C \int_{\mathbb{R}^3} |\rho_{\mathcal{D}_j}^{1+\beta_\pm} - \rho_{\mathcal{D}}^{1+\beta_\pm}|\, d\mathbf{r} \\ &\leq C\Big(\int |\rho_{\mathcal{D}_j} - \rho_{\mathcal{D}}|^{1/(1-\beta_\pm)}\Big)^{1-\beta_\pm} \Big(\int (\rho_{\mathcal{D}_j}^{\beta_\pm} + \rho_{\mathcal{D}}^{\beta_\pm})^{1/\beta_\pm}\Big)^{\beta_\pm}. \end{aligned}$$

Using the Sobolev embedding $\mathbf{H}^{1/2} \hookrightarrow L^r(\mathbb{R}^3)$, $2 \leq 2r \leq 3$, we have that

$$\begin{aligned} \|\rho_{\mathcal{D}_j} - \rho_{\mathcal{D}}\|_{L^r(\mathbb{R}^3)} &\leq C\Big(\int |\sqrt{\rho_{\mathcal{D}_j}} - \sqrt{\rho_{\mathcal{D}}}|^{2r}\Big)^{1/r} \\ &\leq C\|\sqrt{\rho_{\mathcal{D}_j}} - \sqrt{\rho_{\mathcal{D}}}\|_{\mathbf{H}^1}^2. \end{aligned}$$

Since $\|\mathcal{D}_j - \mathcal{D}\|_{\mathcal{H}} \to 0$, Lemma A.1 implies that $\sqrt{\rho_{\mathcal{D}_j}}$ converges strongly to $\sqrt{\rho_{\mathcal{D}}}$ in $\mathbf{H}^{1/2}(\mathbb{R}^3)$, we have established the continuity of E_{xc}. □

Next we show that minimizing sequences cannot tend to zero.

Lemma 5.3. *Suppose $\lambda > 0$ and let $(\mathcal{D}_j)_{j\in\mathbb{N}}$ be a minimizing sequence for* (4.2)*. Then there exists $R > 0$ such that*

$$\lim_{j\to\infty} \sup_{x\in\mathbb{R}^3} \int_{x+B_R} \rho_{\mathcal{D}_j} > 0.$$

A similar statement is valid for the minimizing sequence for (4.4)*.*

Proof. We argue by contradiction. So, suppose $(\mathcal{D}_j)_{j\in\mathbb{N}}$ is a minimizing sequence for (4.2) such that, for all $R > 0$,

$$\lim_{j\to\infty} \sup_{x\in\mathbb{R}^3} \int_{x+B_R} \rho_{\mathcal{D}_j} = 0. \tag{5.7}$$

In view of Lemma 5.1 $\{\mathcal{D}_j\}$ is a bounded sequence in $\mathcal{H}$ and, in particular, $\{\rho_{\mathcal{D}_j}\}$ is bounded in $\mathbf{H}^{1/2}(\mathbb{R}^3)$. The latter, in conjunction with (5.7) and an application of Proposition 2.1 imply that $\rho_{\mathcal{D}_j}$ converges (strongly) to zero in $L^p(\mathbb{R}^3)$ provided $1 < p < 3/2$. In particular, it follows that

$$\lim_{n\to\infty} \int_{\mathbb{R}^3} E_{\mathrm{xc}}(\rho_{\mathcal{D}_j}) = 0.$$

Indeed, for $r \in (1, 3/2)$ and $r^{-1} + q^{-1} = 1$, Hölder's inequality yields

$$\begin{aligned} |E_{\mathrm{xc}}(\rho_{\mathcal{D}_j})| &\le C \int_{\mathbb{R}^3} \rho_{\mathcal{D}_j}^{1+\beta_\pm}\, d\mathbf{r} \le C\Big(\int \rho_{\mathcal{D}_j}^r\Big)^{1/r}\Big(\int \rho_{\mathcal{D}_j}^{q\beta_\pm}\Big)^{1/q} \\ &\le C\|\rho_{\mathcal{D}_j}\|_{L^r} \to 0, \end{aligned}$$

where we used that $\rho_{\mathcal{D}_j}$ converges (strongly) to zero in $L^p(\mathbb{R}^3)$ provided $1 < p < 3/2$.

For any $\epsilon > 0$ and $R > 0$ chosen such that $|V| \le \epsilon\lambda^{-1}$ on B_R^{c}, we have that, provided n is sufficiently large,

$$\begin{aligned} \Big|\int_{\mathbb{R}^3} V\rho_{\mathcal{D}_j}\Big| &\le \int_{B_R} |V|\rho_{\mathcal{D}_j} + \int_{B_R^{\mathrm{c}}} |V|\rho_{\mathcal{D}_j} \\ &\le \Big(\int_{B_R} |V|^{p'}\Big)^{1/p'}\Big(\int_{B_R} \rho_{\mathcal{D}_j}^p\Big)^{1/p} + \frac{\epsilon}{\lambda}\int_{B_R^{\mathrm{c}}} \rho_{\mathcal{D}_j} \le 2\epsilon. \end{aligned}$$

where, once again, we used that $\rho_{\mathcal{D}_j}$ converges (strongly) to zero in $L^p(\mathbb{R}^3)$ provided $1 < p < 3/2$ and $V \in L^q + L^{q'}$ is clearly fulfilled for $3 < q, q' < \infty$. Hence

$$\lim_{j\to\infty} \int_{\mathbb{R}^3} V\rho_{\mathcal{D}_j} = 0.$$

Since

$$\mathcal{E}(\rho_{\mathcal{D}_j}) \ge \int_{\mathbb{R}^3} V\rho_{\mathcal{D}_j} + E_{\mathrm{xc}}(\rho_{\mathcal{D}_j})$$

we find that $I_\lambda \ge 0$ but this contradicts the previously proved result, $I_\lambda < 0$. Hence we conclude that $(\rho_{\mathcal{D}_j})_{j\in\mathbb{N}}$ cannot vanish. The analogous problem in (4.2) is easier to treat because the energy functional contains a single nonpositive term, namely $E_{\mathrm{xc}}(\rho)$. $\square$

Lemma 5.4. *Suppose* $(\alpha_n)_{n\in\mathbb{N}}$ *is a sequence of positive numbers that converges to* 1*, and let* $(\rho_k)_{k\in\mathbb{N}}$ *be a sequence of nonnegative densities such that* $(\sqrt{\rho_n})_{n\in\mathbb{N}}$ *is bounded in* $\mathbf{H}^{1/2}(\mathbb{R}^3)$*. Then*

$$\lim_{k\to\infty}[E_{\mathrm{xc}}(\alpha_k\rho_k) - E_{\mathrm{xc}}(\rho_k)] = 0.$$

Proof. Assumption 1.1 implies that there exists $1 < p_- \le p_+ < 5/3$ and $C \in \mathbb{R}_+$ such that, provided k is sufficiently large,

$$|E_{\mathrm{xc}}(\alpha_k\rho_k) - E_{\mathrm{xc}}(\rho_k)| \le C|\alpha_k - 1| \int_{\mathbb{R}^3} (\rho_k^{p_-} + \rho_k^{p_+}).$$

Since $(\sqrt{\rho_k})_{k\in\mathbb{N}}$ is bounded in $\mathbf{H}^{1/2}(\mathbb{R}^3)$, $(\rho_k)_{k\in\mathbb{N}}$ is bounded in $L^p(\mathbb{R}^3)$ for all $1 \le p \le 3/2$, and $(T_0^{1/2}\sqrt{\rho_k})_{k\in\mathbb{N}}$ is bounded in $(L^2(\mathbb{R}^3))^3$, the result follows. □

With these preparations we are ready to establish concentration-compactness type inequalities.

Proposition 5.5. *Let Assumption 1.1 be satisfied. Then the minimization problems in* (4.2) *and* (4.4) *have the following properties:*

(1) $I_0 = I_0^\infty = 0$ *and for all* $\lambda > 0$*, one has* $-\infty < I_\lambda < I_\lambda^\infty < 0$*;*
(2) *For all* $0 < \mu < \lambda$*, one has*

$$I_\lambda \le I_\mu + I_{\lambda-\mu}^\infty\,; \tag{5.8}$$

The functions $\lambda \mapsto I_\lambda$ *and* $\lambda \mapsto I_\lambda^\infty$ *are continuous and decreasing.*

Proof. Evidently, $I_0 = I_0^\infty$ and $I_\lambda \le I_\lambda^\infty$ for any $\lambda \in \mathbb{R}_+$. Next we establish assertion 2.

Let $\epsilon > 0$, $0 < \mu < \lambda$, and let $\mathcal{D} \in \mathcal{K}_\mu$ such that $I_\mu \le \mathcal{E}(\mathcal{D}) \le I_\mu + \epsilon$. As a consequence of Lemma A.1 we may choose, without loss of generality, $\mathcal{D}$ on the form

$$\mathcal{D} = \sum_{n=1}^N \nu_n\,|\phi_n\rangle\langle\phi_n|$$

with $\nu_n \in [0,1]$, $\sum_{n=1}^N \nu_n = \mu$, $\langle\phi_m,\phi_n\rangle = \delta_{mn}$, $\phi_n \in C_0^\infty(\mathbb{R}^3)$. Indeed, the finite-rank operators in $\mathcal{H}$ are dense and $C_0^\infty(\mathbb{R}^3)$ is dense in $L^2(\mathbb{R}^3)$. Similarly, there exists

$$\widetilde{\mathcal{D}} = \sum_{n=1}^N \tilde{\nu}_n\,|\tilde{\phi}_n\rangle\langle\tilde{\phi}_n|$$

with $\tilde{\nu}_n \in [0,1]$, $\sum_{n=1}^N \tilde{\nu}_n = \lambda - \mu$, $\langle\tilde{\phi}_m,\tilde{\phi}_n\rangle = \delta_{mn}$, $\tilde{\phi}_n \in C_0^\infty(\mathbb{R}^3)$ and satisfying

$$I_{\lambda-\mu}^\infty \le \mathcal{E}^\infty(\widetilde{\mathcal{D}}) \le I_{\lambda-\mu}^\infty + \epsilon.$$

Let $\mathbf{e}$ be a unit vector of $\mathbb{R}^3$ and let $\mathcal{T}_{\mathbf{a}}$ be the translation operator on $L^2(\mathbb{R}^3)$ defined by $\mathcal{T}_{\mathbf{a}}f = f(\cdot - \mathbf{a})$ for any $f \in L^2(\mathbb{R}^3)$. Define, for $j \in \mathbb{N}$,

$$\mathcal{D}_j = \mathcal{D} + \mathcal{T}_{j\mathbf{e}}\widetilde{\mathcal{D}}\mathcal{T}_{-j\mathbf{e}}.$$

For j large enough, we see that $\mathcal{D}_j \in \mathcal{K}_\lambda$ and, using the Pauli principle,

$$I_\lambda \le \mathcal{E}(\mathcal{D}_j) \le \mathcal{E}(\mathcal{D}) + \mathcal{E}^\infty(\widetilde{\mathcal{D}}) + 2\mathcal{J}(\rho_{\mathcal{D}}, \mathcal{T}_{j\mathbf{e}}\rho_{\widetilde{\mathcal{D}}}) \le I_\mu + I^\infty_{\lambda-\mu} + 3\epsilon,$$

whence (5.8). By analogous reasoning, we also show that

$$I^\infty_\lambda \le I^\infty_\mu + I^\infty_{\lambda-\mu}. \tag{5.9}$$

Next, following Le Bris [12, p 122] we consider a L^2-normalized function $\phi \in C_0^\infty(\mathbb{R}^3)$. For all $\sigma > 0$ and all $\lambda \in [0,1]$, the density operator $\mathcal{D}_{\sigma,\lambda}$ with density matrix given by

$$\mathcal{D}_{\sigma,\lambda}(\mathbf{r}, \mathbf{r}') = \lambda\sigma^3\phi(\sigma\mathbf{r})\phi(\sigma\mathbf{r}')$$

belongs to $\mathcal{K}_\lambda$.

In view of (1.11), we infer that there exists $1 \le \gamma < 3/2$, $c > 0$ and $\sigma_0 > 0$ such that for all $\lambda \in [0,1]$ and all $\sigma \in [0, \sigma_0]$, the estimate

$$I^\infty_\lambda \le \mathcal{E}^\infty(\mathcal{D}_{\sigma,\lambda}) \le \lambda\sigma^2\tilde{\mathfrak{t}}_0[\phi,\phi] + \lambda^2\sigma\mathcal{J}(2|\phi|^2) - c\lambda^\gamma\sigma^{3\gamma-1}\int_{\mathbb{R}^3}|\phi|^{2\gamma}.$$

Hence $I^\infty_\lambda < 0$ provided $\lambda > 0$ is sufficiently small. As a consequence of (1.11) and (5.9), the functions $\lambda \mapsto I_\lambda$ and $\lambda \mapsto I^\infty_\lambda$ are decreasing and, for any positive λ, we conclude that

$$-\infty < I_\lambda \le I^\infty_\lambda < 0.$$

Next we prove that $I_\lambda < I^\infty_\lambda$ and therefore we consider a minimizing sequence $(\mathcal{D}_j)_{j\in\mathbb{N}}$ for (4.4). An application of Lemma 5.3 ensures the existence of $\eta > 0$ and $R > 0$ such that for j large enough, there exists $\mathbf{r}_j \in \mathbb{R}^3$ so that

$$\int_{\mathbf{r}_j + B_R} \rho_{\mathcal{D}_j} \ge \eta$$

We define $\widetilde{\mathcal{D}}_j = \mathcal{T}_{\mathbf{R}_1 - \mathbf{r}_j}\mathcal{D}_j\mathcal{T}_{\mathbf{r}_j - \mathbf{R}_1}$. Then $\widetilde{\mathcal{D}}_j \in \mathcal{K}_\lambda$ and

$$\mathcal{E}(\widetilde{\mathcal{D}}_j) \le \mathcal{E}^\infty(\mathcal{D}_j) - \frac{Z_1\alpha\eta}{R}.$$

Hence

$$I_\lambda \le I^\infty_\lambda - \frac{Z_1\alpha\eta}{R} < I^\infty_\lambda.$$

To prove that the functions $\lambda \mapsto I_\lambda$ and $\lambda \mapsto I^\infty_\lambda$ are continuous, we will apply Lemma 5.4. We establish left-continuity of $\lambda \mapsto I_\lambda$. Let $\lambda > 0$, and let $(\lambda_k)_{k\in\mathbb{N}}$ be an increasing sequence of positive real numbers converging to λ. Let $\epsilon > 0$ and $\mathcal{D} \in \mathcal{K}_\lambda$ such that

$$I_\lambda \le \mathcal{E}(\mathcal{D}) \le I_\lambda + \frac{\epsilon}{2}.$$

For all $k \in \mathbb{N}$, $\mathcal{D}_k = \lambda_k \lambda^{-1} \mathcal{D}$ in $\mathcal{K}_{\lambda_k}$ so that for all $k \in \mathbb{N}$ and all $n \in \mathbb{N}$,

$$I_\lambda \le I_{\lambda_k} \le \mathcal{E}(\mathcal{D}_k).$$

Furthermore, by virtue of Lemma 5.4, we have that

$$\begin{aligned}\mathcal{E}(\mathcal{D}_k) = \frac{\lambda_k}{\lambda}\alpha^{-1}\operatorname{Tr}(\widetilde{T}_0\mathcal{D}) + \frac{\lambda_k}{\lambda}\alpha^{-1}\int_{\mathbb{R}^3} V\rho_{\mathcal{D}} \\ + \frac{\lambda_k}{\lambda^2}\mathcal{J}(\rho_{\mathcal{D}}) + E_{\mathrm{xc}}\big(\frac{\lambda_k}{\lambda}\rho_{\mathcal{D}}\big) \underset{k\to\infty}{\longrightarrow} \mathcal{E}(\mathcal{D}).\end{aligned}$$

Hence, for k large enough,

$$I_\lambda \le I_{\lambda_k} \le I_\lambda + \epsilon$$

We proceed to establishing the right-continuity of $\lambda \mapsto I_\lambda$. Let $\lambda > 0$, and let $(\lambda_k)_{k\in\mathbb{N}}$ be a decreasing sequence of positive real numbers converging to λ. For each $k \in \mathbb{N}$ we select $\mathcal{D}_k \in \mathcal{K}_{\lambda_k}$ such that

$$I_{\lambda_k} \le \mathcal{E}(\mathcal{D}_{\lambda_k}) \le I_{\lambda_k} + \frac{1}{k}.$$

For all $k \in \mathbb{N}$, we define $\widetilde{\mathcal{D}}_k = \lambda\lambda_k^{-1}\mathcal{D}_k$. Since $\widetilde{\mathcal{D}}_k \in \mathcal{K}_{\lambda_k}$ we find that

$$I_{\lambda_k} \le \mathcal{E}(\widetilde{\mathcal{D}}_k) = \frac{\lambda}{\lambda_k}\operatorname{Tr}(T_0\mathcal{D}_k) + \frac{\lambda}{\lambda_k}\int_{\mathbb{R}^3} V\rho_{\mathcal{D}_k} + \frac{\lambda}{\lambda_k^2}\mathcal{J}(\rho_{\mathcal{D}_k}) + E_{\mathrm{xc}}\big(\frac{\lambda}{\lambda_k}\rho_{\mathcal{D}_k}\big).$$

Since $(\mathcal{D}_k)_{k\in\mathbb{N}}$ is bounded in $\mathcal{H}$ and $(\sqrt{\rho_{\mathcal{D}_k}})_{k\in\mathbb{N}}$ is bounded in $\mathbf{H}^{1/2}(\mathbb{R}^3)$, an application of Lemma 5.4 yields

$$\lim_{k\to\infty}\Big(\mathcal{E}(\widetilde{\mathcal{D}}_k) - \mathcal{E}(\mathcal{D}_k)\Big) = 0.$$

Take $\epsilon > 0$ and $k_\epsilon \ge 2\epsilon^{-1}$ such that for all $k \ge k_\epsilon$,

$$\big|\mathcal{E}(\widetilde{\mathcal{D}}_k) - \mathcal{E}(\mathcal{D}_k)\big| \le \frac{\epsilon}{2}.$$

Then

$$\forall k \ge k_\epsilon, \quad I_\lambda - \epsilon \le I_{\lambda_k} \le I_\lambda$$

which shows the right-continuity of $\lambda \mapsto I_\lambda$ on $\mathbb{R}_+ \setminus \{0\}$. Finally, the estimates in Lemma 5.1 imply that $\lim_{\lambda\to 0^+} I_\lambda = 0$. □

6. Decreasing property

Weakly lower semicontinuity is not valid in the usual sense. However, the following result suffices for our purpose.

Lemma 6.1. *Let $(\mathcal{D}_j)_{j\in\mathbb{N}}$ be a sequence in $\mathcal{K}$, bounded in $\mathcal{H}$, such that $\mathcal{D}_j \to \mathcal{D}$ in the weak-$*$ topology of $\mathcal{H}$. If $\lim_{j\to\infty}\operatorname{Tr}(\mathcal{D}_j) = \operatorname{Tr}(\mathcal{D})$, then $\rho_{\mathcal{D}_j} \to \rho_{\mathcal{D}}$ strongly in $L^p(\mathbb{R}^3)$ for all $p \in [1, 3/2)$, and*

$$\mathcal{E}(\mathcal{D}) \le \liminf_{j\to\infty}\mathcal{E}(\mathcal{D}_j),$$

$$\mathcal{E}^\infty(\mathcal{D}) \le \liminf_{j\to\infty}\mathcal{E}^\infty(\mathcal{D}_j).$$

Proof. Bear in mind that $(\mathcal{D}_j)_{j\in\mathbb{N}}$ converges to $\mathcal{D}$ in the weak-$*$ topology of $\mathcal{H}$ means that, for any compact K on $L^2(\mathbb{R}^3)$,

$$\lim_{j\to\infty} \mathrm{Tr}(\mathcal{D}_j K) = \mathrm{Tr}(\mathcal{D}K), \quad \lim_{j\to\infty} \mathrm{Tr}(T_0^{1/2}\mathcal{D}_j T_0^{1/2}K) = \mathrm{Tr}(T_0^{1/2}\mathcal{D}T_0^{1/2}K).$$

In view of (3.4) we introduce $P_+(\alpha)$ as the projection onto the pure point spectral subspace of $H_{1,1,\alpha}$ in $\mathfrak{H} := L^2(\mathbb{R}^3)$ and we let $P_-(\alpha) = 1 - P_+(\alpha)$. Then, following the idea in [4, p 141], we decompose the functional $\mathcal{E}(\cdot)$ into three terms

$$\alpha\mathcal{E}(\mathcal{D}_j) = P_1(\mathcal{D}_j) + P_2(\mathcal{D}_j) + \mathcal{L}(\mathcal{D}_j), \tag{6.1}$$

where

$$P_1(\mathcal{D}_j) = \mathrm{Tr}\left[P_+(\alpha)H_{1,1,\alpha}P_+(\alpha)\mathcal{D}_j\right], \tag{6.2}$$
$$P_2(\mathcal{D}_j) = \mathrm{Tr}\left[P_-(\alpha)H_{1,1,\alpha}P_-(\alpha)\mathcal{D}_j\right], \tag{6.3}$$
$$\mathcal{L}(\mathcal{D}_j) = \frac{1}{2}\left(\mathcal{J}(\mathcal{D}_j) - E_{\mathrm{xc}}(\mathcal{D}_j)\right). \tag{6.4}$$

Step 1. We begin by proving that $P_1(\mathcal{D}) \le \liminf_j P_1(\mathcal{D}_j)$. We select an orthonormal basis $\{e_k\}$ in $\mathfrak{H} = L^2(\mathbb{R}^3)$ such that $e_k \in \mathbf{H}^{1/2}(\mathbb{R}^3)$. Moreover, we introduce the functions

$$\psi_k = [P_+(\alpha)H_{1,1,\alpha}P_+(\alpha)]^{1/2}e_k$$

If $\langle\cdot,\cdot\rangle$ denotes the scalar product in $\mathfrak{H}$, then the weak convergence in $\mathfrak{S}_2(\mathfrak{H})$ implies

$$\begin{aligned} P_1(\mathcal{D}_j) &= \mathrm{Tr}\left([P_+(\alpha)H_{1,1,\alpha}P_+(\alpha)]^{1/2}\mathcal{D}_j[P_+(\alpha)H_{1,1,\alpha}P_+(\alpha)]^{1/2}\right) \\ &= \sum_k \langle\psi_k\mathcal{D}_j\psi_k\rangle \\ &= \sum_k \langle T_0^{-1/2}\psi_k, \widetilde{D}^{(j)}T_0^{-1/2}\psi_k\rangle \end{aligned}$$

where $\widetilde{\mathcal{D}}^{(j)} = T_0^{1/2}\mathcal{D}_jT_0^{1/2}$. An application of Fatou's lemma, together with the nonnegativity of the Hilbert-Schmidt operator

$$T_k = \langle\cdot, T_0^{-1/2}\psi_k\rangle T_0^{-1/2}\psi_k$$

and the hypothesis yield

$$\liminf_{j\to\infty} P_1(\mathcal{D}_j) = \liminf_{j\to\infty}\sum_k \mathrm{Tr}[T_k\widetilde{\mathcal{D}}^{(j)}] \ge \sum_k \mathrm{Tr}[T_k\widetilde{\mathcal{D}}] = P_1(\mathcal{D}).$$

A similar argument is found in [21, 4, 5].

Step 2. Since $P_-(\alpha)H_{1,1,\alpha}P_-(\alpha)$ is a Hilbert-Schmidt operator (see, e.g., [5]) and thus compact, we immediately obtain

$$\begin{aligned} \lim_{j\to\infty} P_2(\mathcal{D}_j) &= \lim_j \mathrm{Tr}[P_-(\alpha)H_{1,1,\alpha}P_-(\alpha)\mathcal{D}_j] \\ &= \mathrm{Tr}[P_-(\alpha)H_{1,1,\alpha}P_-(\alpha)\mathcal{D}] = P_2(\mathcal{D}_J). \end{aligned}$$

Step 3. We have seen that $(\sqrt{\rho_{\mathcal{D}_j}})_{j\in\mathbb{N}}$ is a bounded sequence in $\mathbf{H}^{1/2}(\mathbb{R}^3)$, so $\sqrt{\rho_{\mathcal{D}_j}} \to \sqrt{\rho_{\mathcal{D}}}$ weakly in $\mathbf{H}^{1/2}(\mathbb{R}^3)$ and strongly in $L^p(\mathbb{R}^3)$ for all $p \in [2,3)$. In particular, $\sqrt{\rho_{\mathcal{D}_j}}$ converges weakly to $\sqrt{\rho_{\mathcal{D}}}$ in $L^2(\mathbb{R}^3)$. On the other hand, we know that

$$\begin{aligned}\lim_{j\to\infty} \|\sqrt{\rho_{\mathcal{D}_j}}\|_{L^2}^2 &= \lim_{j\to\infty} \int_{\mathbb{R}^3} \rho_{\mathcal{D}_j} = 2 \lim_{j\to\infty} \operatorname{Tr}(\mathcal{D}_j) \\ &= 2\operatorname{Tr}(\mathcal{D}) = \int_{\mathbb{R}^3} \rho_{\mathcal{D}} = \|\sqrt{\rho_{\mathcal{D}}}\|_{L^2}^2.\end{aligned}$$

We conclude that $\sqrt{\rho_{\mathcal{D}_j}} \to \sqrt{\rho_{\mathcal{D}}}$ strongly in $L^2(\mathbb{R}^3)$. A standard bootstrap argument, using that $\|\sqrt{\rho_{\mathcal{D}_j}}\|_{L^p} < C$ for any $2 \le p \le 3$ and interpolation, implies that $\{\sqrt{\rho_{\mathcal{D}_j}}\}_{j\in\mathbb{N}}$ converges strongly to $\sqrt{\rho_{\mathcal{D}}}$ in $L^p(\mathbb{R}^3)$ for all $p \in [2,3)$ and, consequently, $\{\rho_{\mathcal{D}_j}\}_{j\in\mathbb{N}}$ converges to $\rho_{\mathcal{D}}$ strongly in $L^p(\mathbb{R}^3)$ for all $p \in [1,3/2)$. We immediately obtain

$$\lim_{j\to\infty} \mathcal{J}(\rho_{\mathcal{D}_j}) = \mathcal{J}(\rho_{\mathcal{D}}), \quad \lim_{j\to\infty} E_{\mathrm{xc}}(\rho_{\mathcal{D}_j}) = E_{\mathrm{xc}}(\rho_{\mathcal{D}}).$$

Indeed,

$$\begin{aligned}&|J(\rho_{\mathcal{D}_j}) - J(\rho_{\mathcal{D}})| \\ &= \left|\frac{1}{2}\int [(\rho_{\mathcal{D}_j} - \rho_{\mathcal{D}}) * W](\rho_{\mathcal{D}_j} + \rho_{\mathcal{D}})\,dx\right| \\ &\le C\|\rho_{\mathcal{D}_j} - \rho_{\mathcal{D}}\|_{L^1}\Big(\|W_1\|_{L^4}\|\rho_{\mathcal{D}_j} + \rho_{\mathcal{D}}\|_{L^{4/3}} + \|W_2\|_{L^\infty}\|\rho_{\mathcal{D}_j} + \rho_{\mathcal{D}}\|_{L^1}\Big)\end{aligned}$$

and the claim thus follows from the afore-mentioned strong convergence. Similarly, Hölder's inequality and the strong convergence yield

$$\begin{aligned}&|E_{\mathrm{xc}}(\rho_{\mathcal{D}_j}) - E_{\mathrm{xc}}(\rho_{\mathcal{D}})| \\ &\le C\int |\rho_{\mathcal{D}_j} - \rho_{\mathcal{D}}|(\rho_{\mathcal{D}_j}^{\beta_\pm} + \rho_{\mathcal{D}}^{\beta_\pm})\,d\mathbf{r} \\ &\le C\Big(\int |\rho_{\mathcal{D}_j} - \rho_{\mathcal{D}}|^{1/(1-\beta_\pm)}\Big)^{1-\beta_\pm}\Big(\int (\rho_{\mathcal{D}_j}^{\beta_\pm} + \rho_{\mathcal{D}}^{\beta_\pm})^{1/\beta_\pm}\Big)^{\beta_\pm} \underset{j\to\infty}{\longrightarrow} 0.\end{aligned}$$

□

Arguments similar to those in Steps 1 and 2 are found in [21, 4, 5, 8].

7. Proof of main result

Proof of Theorem 1.2. It follows from Lemma 5.1 that $\mathcal{E}(\cdot)$ is bounded from below. Let $(\mathcal{D}_j)_{j\in\mathbb{N}}$ be a minimizing sequence for I_λ. Then Lemma 5.1 also shows that $(\mathcal{D}_j)_{j\in\mathbb{N}}$ is bounded in $\mathcal{H}$ and that $(\sqrt{\rho_{\mathcal{D}_j}})_{j\in\mathbb{N}}$ is bounded in $\mathbf{H}^{1/2}(\mathbb{R}^3)$. By extracting a suitable subsequence, again denoted by $(\mathcal{D}_j)_{j\in\mathbb{N}}$, we may assume that $(\mathcal{D}_j)_{j\in\mathbb{N}}$ converges to some $\mathcal{D} \in \mathcal{K}$ for the weak-$*$ topology of $\mathcal{H}$ and that $(\sqrt{\rho_{\mathcal{D}_j}})_{j\in\mathbb{N}}$ converges to $\sqrt{\rho_{\mathcal{D}}}$ weakly in $\mathbf{H}^{1/2}(\mathbb{R}^3)$, strongly in $L^p_{\mathrm{loc}}(\mathbb{R}^3)$ for all $2 \le p < 3$ and almost everywhere.

Case $\mathrm{Tr}(\mathcal{D}) = \lambda$. Evidently, $\lambda \in \mathcal{K}_\lambda$ and Lemma 6.1 yields

$$\mathcal{E}(\mathcal{D}) \leq \liminf_{j\to\infty} \mathcal{E}(\mathcal{D}_j) = I_\lambda,$$

whence $\mathcal{D}$ is a minimizer of (4.2).
Case $\mathrm{Tr}(\mathcal{D}) < \lambda$. Define $\vartheta := \mathrm{Tr}(\mathcal{D})$ and suppose that $0 < \vartheta < \lambda$. Let χ be a smooth, radial function, non-increasing in the radial direction, which satisfies $\chi(0) = 1$, $0 \leq \chi(x) < 1$ if $|x| > 0$, $\chi(x) = 0$ if $|x| \geq 1$, $\|\nabla\chi\|_{L^\infty} \leq 2$ and $\|\nabla(1-\chi^2)^{1/2}\|_{L^\infty} \leq 2$. Introduce the quadratic partition of unity $\chi^2 + \zeta^2 = 1$ and put $\chi_R(\cdot) = \chi(\cdot/R)$. For any $j \in \mathbb{N}$, $R \mapsto \mathrm{Tr}(\chi_R \mathcal{D}_j \chi_R)$ is a continuous nondecreasing function which equals zero at $R = 0$ and $\lim_{R\to\infty} \mathrm{Tr}(\chi_R \mathcal{D}_j \chi_R) = \mathrm{Tr}(\mathcal{D}_j) = \lambda$. Choose $R_j > 0$ such that $\mathrm{Tr}(\chi_{R_j} \mathcal{D} \chi_{R_j}) = \vartheta$. Then $R_j \to \infty$, otherwise $(R_j)_{j\in\mathbb{N}}$ contains a subsequence which converges to some (finite value) $\tilde{R}$ and, consequently,

$$\begin{aligned}
\int_{\mathbb{R}^3} \rho_{\mathcal{D}}(x)\chi_{\tilde{R}}^2(x)\,dx &= \lim_{k\to\infty} \int_{\mathbb{R}^3} \rho_{\mathcal{D}_{j_k}}(x)\chi_{R_{j_k}}^2\,dx \\
&= 2\lim_{k\to\infty} \mathrm{Tr}(\chi_{R_{j_k}} \mathcal{D}_{j_k} \chi_{R_{j_k}}) \\
&= 2\vartheta = \int_{\mathbb{R}^3} \rho_{\mathcal{D}}(x)\,dx
\end{aligned}$$

Since $\chi_{\tilde{R}}^2 < 1$ on $\mathbb{R}^3 \setminus \{0\}$ we obtain a contradiction. As a consequence, $(R_j)_{j\in\mathbb{N}}$ goes to infinity. Next we introduce

$$\mathcal{D}_{1,j} = \chi_{R_j} \mathcal{D}_j \chi_{R_j}, \quad \mathcal{D}_{2,j} = \zeta_{R_j} \mathcal{D}_j \zeta_{R_j}$$

Then:

(1) $0 \leq \mathcal{D}_{i,j} \leq 1$;
(2) $\mathcal{D}_{i,j}$ are trace class self-adjoint operators on $L^2(\mathbb{R}^3)$;
(3) $\rho_{\mathcal{D}_j} = \rho_{\mathcal{D}_{1,j}} + \rho_{\mathcal{D}_{2,j}}$; and
(4) $\mathrm{Tr}(\mathcal{D}_{1,j}) = \vartheta$, $\quad \mathrm{Tr}(\mathcal{D}_{2,j}) = \lambda - \vartheta$.

The following IMS-type estimate

$$T_0 \geq \chi_{R_j} T_0 \chi_{R_j} + \zeta_{R_j} T_0 \zeta_{R_j} - \frac{1}{\pi}\int_0^\infty \frac{1}{T_0^2+\tau}\left(|\nabla\chi_{R_j}|^2 + |\nabla\zeta_{\mathbb{R}_j}|^2\right)\frac{1}{T_0^2+\tau}\sqrt{\tau}\,d\tau$$

is useful at this stage; see Lemma 3.1. Employing $\|\nabla\chi_{R_j}\|_{L^\infty}^2 + \|\nabla\zeta_{R_j}\|_{L^\infty}^2 \leq C/R^2$ and the uniform boundedness of $\mathrm{Tr}(\mathcal{D}_j)$, we obtain

$$\mathrm{Tr}(T_0\mathcal{D}_j) \geq \mathrm{Tr}(T_0\mathcal{D}_{1,j}) + \mathrm{Tr}(T_0\mathcal{D}_{2,j}) - \frac{c\lambda}{R_j^2} \tag{7.1}$$

We infer that the sequences $(\mathcal{D}_{1,j})_{j\in\mathbb{N}}$ and $(\mathcal{D}_{2,j})_{j\in\mathbb{N}}$ are bounded on $\mathcal{H}$. For any $\phi \in C_0^\infty(\mathbb{R}^3)$, we have that

$$\begin{aligned}
\operatorname{Tr}\left(\mathcal{D}_{1,j}\,|\phi\rangle\langle\phi|\,\right) &= \operatorname{Tr}\left(\mathcal{D}_{1,j}\left(\,|\xi_{R_j}\phi\rangle\langle\xi_{R_j}\phi|\,\right)\right)\\
&= \operatorname{Tr}\left(\mathcal{D}_{1,j}\left(\,|(\xi_{R_j}-1)\phi\rangle\langle\xi_{R_j}\phi|\,\right)\right) + \operatorname{Tr}\left(\mathcal{D}_j\left(\,|\phi\rangle\langle(\xi_{R_j}-1)\phi|\,\right)\right)\\
&\quad + \operatorname{Tr}\left(\mathcal{D}_j\left(\,|\phi\rangle\langle\phi|\,\right)\right)\\
&\underset{j\to\infty}{\longrightarrow} \operatorname{Tr}\left(\mathcal{D}\left(\,|\phi\rangle\langle\phi|\,\right)\right),
\end{aligned}$$

which shows that $(\mathcal{D}_{1,j})_{j\in\mathbb{N}}$ converges to $\mathcal{D}$ for the weak-$*$ topology of $\mathcal{H}$. Since $\operatorname{Tr}(\mathcal{D}_{1,j}) = \vartheta = \operatorname{Tr}(\mathcal{D})$ for all j, we infer from Lemma 6.1 that $(\rho_{\mathcal{D}_{1,j}})$ converges to $\rho_{\mathcal{D}}$ strongly in $L^p(\mathbb{R}^3)$, $p\in[1,3/2)$, and

$$\mathcal{E}(\mathcal{D}) \le \lim_{j\to\infty} \mathcal{E}(\mathcal{D}_{1,j}) \tag{7.2}$$

because $\rho_{\mathcal{D}_{2,j}} = \rho_{\mathcal{D}_j} - \rho_{\mathcal{D}_{1,j}}$. In particular, $(\rho_{\mathcal{D}_{2,j}})$ converges strongly to zero in $L^p_{\mathrm{loc}}(\mathbb{R}^3)$, $p\in[1,3/2)$ and $(\rho_{\mathcal{D}_j})$ and $(\rho_{\mathcal{D}_{1,j}})$ converge to $\rho_{\mathcal{D}}$ in L^p_{loc}. Another application of (7.1) yields

$$\begin{aligned}
\mathcal{E}(\mathcal{D}_j) &= \operatorname{Tr}(\widetilde{T}_0\mathcal{D}_j) + \int_{\mathbb{R}^3} V\rho_{\mathcal{D}_j} + \mathcal{J}(\rho_{\mathcal{D}_j}) + \int_{\mathbb{R}^3} g(\rho_{\mathcal{D}_j})\\
&\ge \operatorname{Tr}(\widetilde{T}_0\mathcal{D}_{1,j}) + \operatorname{Tr}(\widetilde{T}_0\mathcal{D}_{2,j}) + \int_{\mathbb{R}^3} V\rho_{\mathcal{D}_{1,j}} + \int_{\mathbb{R}^3} V\rho_{\mathcal{D}_{2,j}} +\\
&\quad + \mathcal{J}(\rho_{\mathcal{D}_{1,j}}) + \mathcal{J}(\rho_{\mathcal{D}_{2,j}}) + \int_{\mathbb{R}^3} g(\rho_{\mathcal{D}_{1,j}} + \rho_{\mathcal{D}_{2,j}}) - \frac{c\lambda}{R_j^2}\\
&= \mathcal{E}(\mathcal{D}_{1,j}) + \mathcal{E}^\infty(\mathcal{D}_{2,j}) + \int_{\mathbb{R}^3} V\rho_{\mathcal{D}_{2,j}}\\
&\quad + \int_{\mathbb{R}^3}\left(g(\rho_{\mathcal{D}_{1,j}} + \rho_{\mathcal{D}_{2,j}}) - g(\rho_{\mathcal{D}_{1,j}}) - g(\rho_{\mathcal{D}_{2,j}})\right) - \frac{c\lambda}{R_j^2}.
\end{aligned}$$

Now, on the one hand, by choosing R large enough, we have that

$$\Big|\int_{\mathbb{R}^3} V\rho_{\mathcal{D}_{2,j}}\Big| \le \alpha Z_{\mathrm{tot}}\Big(\int_{B(0,R)} \rho_{\mathcal{D}_{2,j}}\Big)^{1/2} \|\sqrt{\rho_{\mathcal{D}_{2,j}}}\|_{\mathbf{H}^{1/2}} + \frac{\alpha Z_{\mathrm{tot}}(\lambda-\vartheta)}{R}.$$

Furthermore, for some constant C independent of R and n, we have

$$\begin{aligned}
&\Big|\int_{\mathbb{R}^3}\left(g(\rho_{\mathcal{D}_{1,j}} + \rho_{\mathcal{D}_{2,j}}) - g(\rho_{\mathcal{D}_{1,j}}) - g(\rho_{\mathcal{D}_{2,j}})\right)\Big|\\
&\le C\Big\{\int_{B_R}\Big(\rho_{\mathcal{D}_{2,j}} + \rho^2_{\mathcal{D}_{2,j}}\Big) + \|\rho_{\mathcal{D}_{1,j}}\|_{L^2}\Big(\int_{B_R^c} \rho^2_{\mathcal{D}_{2,j}}\Big)^{1/2}\Big\} + C\Big(\int_{B_R} \rho^{p_-}_{\mathcal{D}_{2,j}} + \rho^{p_+}_{\mathcal{D}_{2,j}}\Big)\\
&\quad + C\Big\{\int_{B_R^c}\Big(\rho_{\mathcal{D}_{1,j}} + \rho^2_{\mathcal{D}_{1,j}}\Big) + \|\rho_{\mathcal{D}_{2,j}}\|_{L^2}\Big(\int_{B_R^c} \rho^2_{\mathcal{D}_{1,j}}\Big)^{1/2}\Big\}\\
&\quad + C\Big(\int_{B_R^c} \rho^{p_-}_{\mathcal{D}_{1,j}} + \rho^{p_+}_{\mathcal{D}_{1,j}}\Big)
\end{aligned}$$

We already know that the sequences $(\sqrt{\rho_{\mathcal{D}_{1,j}}})_{n\in\mathbb{N}}$ and $(\sqrt{\rho_{\mathcal{D}_{2,j}}})_{j\in\mathbb{N}}$ are bounded in $\mathbf{H}^{1/2}(\mathbb{R}^3)$, that $\rho_{\mathcal{D}_{1,j}} \to \rho_{\mathcal{D}}$ in $L^p(\mathbb{R}^3)$ for any $p\in[1,3/2)$

and that $\rho_{\mathcal{D}_{2,j}} \to 0$ in $L^p_{\mathrm{loc}}(\mathbb{R}^3)$ for any $p \in [1, 3/2)$. Therefore, for all $\epsilon > 0$, there exists $J \in \mathbb{N}$ such that $\forall j \geq J$,

$$\mathcal{E}(\mathcal{D}_j) \geq \mathcal{E}(\mathcal{D}_{1,j}) + \mathcal{E}^\infty(\mathcal{D}_{2,j}) - \epsilon \geq I_\vartheta + I^\infty_{\lambda-\vartheta} - \epsilon.$$

By letting j tend to infinity, ϵ tend to zero, and applying (5.8), we get that $I_\lambda = I_\vartheta + I^\infty_{\lambda-\vartheta}$ and that $(\mathcal{D}_{1,j})_{j\in\mathbb{N}}$, respectively $(\mathcal{D}_{2,j})_{j\in\mathbb{N}}$ is a minimizing sequence for I_ϑ, respectively for $I^\infty_{\lambda-\vartheta}$. From (7.2); i.e., $\mathcal{E}(\mathcal{D}) \leq \lim_{j\to\infty} \mathcal{E}(\mathcal{D}_{1,j})$, it is seen that $\mathcal{D}$ is a minimizer for I_ϑ.

We take a closer look at the sequence $(\mathcal{D}_{2,j})_{j\in\mathbb{N}}$. Since it is a minimizing sequence for $I^\infty_{\lambda-\vartheta}$, the sequence $(\rho_{\mathcal{D}_j})_{j\in\mathbb{N}}$ cannot vanish. Therefore, there exist $\eta > 0$, $R > 0$ such that, for all $j \in \mathbb{N}$,

$$\int_{y_j + B_R} \rho_{\mathcal{D}_{2,j}} \geq \eta$$

for some $y_j \in \mathbb{R}^3$ and, as a consequence, the sequence $(\mathcal{T}_{y_j}\mathcal{D}_{2,j}\mathcal{T}_{-y_j})_{j\in\mathbb{N}}$ converges in the weak-$*$ topology of $\mathcal{H}$ to some $\widetilde{\mathcal{D}} \in \mathcal{K}$ satisfying $\mathrm{Tr}(\widetilde{\mathcal{D}}) \geq \eta > 0$. By setting $\kappa = \mathrm{Tr}(\widetilde{\mathcal{D}})$ we may argue as above to verify that $\widetilde{\mathcal{D}}$ is a minimizer for I^∞_κ and, in addition,

$$I_\lambda = I_\vartheta + I^\infty_\kappa + I^\infty_{\lambda-\vartheta-\kappa}.$$

However, Proposition A.2 informs us that $I_{\vartheta+\kappa} < I_\vartheta + I^\infty_\kappa$. Hence we conclude that $I_{\vartheta+\kappa} + I^\infty_{\lambda-\vartheta-\kappa} < I_\lambda$ which contradicts Proposition 5.5. This completes the proof. □

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Appendix A. Auxiliary results

We collect some fundamental facts in the following result.

Lemma A.1. *Suppose $\lambda > 0$ and let $\mathcal{D} \in \mathcal{K}_\lambda$. There exists a sequence $\{\mathcal{D}_j\}$ with the following properties:*

(1) *For all $j \in \mathbb{N}$, $\mathcal{D}_j \in \mathcal{K}_\lambda$, $\mathcal{D}_j$ is finite-rank and $\mathrm{Ran}(\mathcal{D}_j) \subset C_0^\infty(\mathbb{R}^3)$;*
(2) *The sequence $\{\mathcal{D}_j\}$ converges to $\mathcal{D}$ strongly in $\mathcal{H}$;*
(3) *The sequence $\{\sqrt{\rho_{\mathcal{D}_j}}\}$ converges to $\sqrt{\rho_{\mathcal{D}}}$ strongly in $\mathbf{H}^{1/2}(\mathbb{R}^3)$;*
(4) *The sequences $\{\rho_{\mathcal{D}_j}\}$ and $\{T_0^{1/2}\sqrt{\rho_{\mathcal{D}_j}}\}$ converge a.e. to $\rho_{\mathcal{D}}$ and $T_0^{1/2}\sqrt{\rho_{\mathcal{D}}}$ respectively.*

Proof. We divide the proof into two steps.
Step 1. Consider $\mathcal{D} \in \mathcal{K}_\lambda$. We have that

$$\mathcal{D} = \sum_{n=1}^{+\infty} \nu_n \, |\phi_n\rangle\langle\phi_n|$$

with $\nu_n \in [0,1]$, $\phi_n \in \mathbf{H}^{1/2}(\mathbb{R}^3)$, $\langle \phi_m, \phi_n\rangle_{L^2} = \delta_{mn}$, $\mathrm{Tr}(\mathcal{D}) = \sum_{n=1}^{+\infty} \nu_n = \lambda$ and $\mathrm{Tr}(T_0\mathcal{D}) = \sum_{n=1}^{+\infty} \nu_n \|T_0^{1/2}\phi_n\|_{L^2}^2 < \infty$.

We begin by verifying that $\mathcal{D}$ can be approximated by a sequence of finite-rank operators. Choose $N_0 \in \mathbb{N}$ such that $n_{N_0} \in (0,1)$; if no such N_0 exists, then $\mathcal{D}$ has finite rank and one can proceed to the second part of the proof without further comments. For all $N \in N$, we introduce

$$\widetilde{\mathcal{D}}_N = \sum_{i=1}^{N} n_i \, |\phi_i\rangle\langle\phi_i| \, + \Big(\lambda - \sum_{i=1}^{N} n_i\Big) \, |\phi_{N_0}\rangle\langle\phi_{N_0}| \, .$$

By choosing N large enough, we have that $\widetilde{\mathcal{D}}_N \in \mathcal{K}_\lambda$ and the sequence $(\widetilde{\mathcal{D}})$ evidently converges to $\mathcal{D}$ in $\mathcal{H}$.

Step 2. Next we show that $\|\widetilde{\mathcal{D}}_N - \mathcal{D}\|_{\mathcal{H}} \to 0$ implies statement 3. First we observe that $(\rho_{\widetilde{\mathcal{D}}_N})$ converges a.e. to $\rho_{\mathcal{D}}$. Second, we have the representation

$$\langle f, \widetilde{T}_0 f\rangle = C \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|f(x)-f(y)|^2}{|x-y|^2} K_2(\alpha^{-1}|x-y|)\, dx\, dy,$$

where $K_2(\cdot)$ is the modified Bessel function of the third kind. We shall show that

$$\big|\langle\sqrt{\rho_{\widetilde{\mathcal{D}}_N}}, \widetilde{T}_0\sqrt{\rho_{\widetilde{\mathcal{D}}_N}}\rangle - \langle\sqrt{\rho_{\mathcal{D}}}, \widetilde{T}_0\sqrt{\rho_{\mathcal{D}}}\rangle\big| \to 0.$$

Since $(\rho_{\widetilde{\mathcal{D}}_N})$ converges a.e. to $\rho_{\mathcal{D}}$, we have

$$\big|\sqrt{\rho_{\widetilde{\mathcal{D}}_N}(x)} - \sqrt{\rho_{\widetilde{\mathcal{D}}_N}(y)}\big|^2 \to \big|\sqrt{\rho_{\mathcal{D}}(x)} - \sqrt{\rho_{\mathcal{D}}(y)}\big|^2 \quad \text{a.e.}$$

Moreover, using Young's inequality, we find that

$$\begin{aligned} &\big|\sqrt{\rho_{\widetilde{\mathcal{D}}_N}(x)} - \sqrt{\rho_{\widetilde{\mathcal{D}}_N}(y)}\big|^2 \\ &\le \big|\sqrt{\rho_{\mathcal{D}}(x)} - \sqrt{\rho_{\mathcal{D}}(y)}\big|^2 + \big|\sqrt{\rho_{\mathcal{D}}(x)} + \sqrt{\rho_{\mathcal{D}}(y)}\big|^2 \end{aligned} \tag{A.1}$$

An application of (5.1) shows that

$$\begin{aligned} &C \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|\sqrt{\rho_{\mathcal{D}}(x)} - \sqrt{\rho_{\mathcal{D}}(y)}|^2}{|x-y|^2} K_2(\alpha^{-1}|x-y|)\, dx\, dy \\ &= \langle\sqrt{\rho_{\mathcal{D}}}, \widetilde{T}_0\sqrt{\rho_{\mathcal{D}}}\rangle \\ &\le \sum_n \nu_n \|\widetilde{T}_0^{1/2}\phi_n\|_{L^2}^2 = \mathrm{Tr}[\widetilde{T}_0\mathcal{D}] < \infty. \end{aligned}$$

This settles the issue of dominance associated with the first term of the right-hand of (A.1), and the second term is taken care of by utilizing the properties of ϕ_n and $K_2(\cdot)$. Hence Lebesgue's dominated convergence theorem allows us to conclude. The final part of the proof amounts to approximating each ϕ_n by a sequence of smooth compactly supported functions. The arguments, which also establishes statement 4, are standard and thus omitted. □

Within the non-relativistic context a similar result was first given by Lions [16, Lemma II.1]. By means of Lemma 3.2 we can prove the following result.

Proposition A.2. *Suppose $\vartheta > 0$ and $vk > 0$ satisfy $\vartheta + \kappa \leq N_{\mathrm{p}} \leq (1/2)Z_{\mathrm{tot}}$. If the problems associated to I_ϑ and I_κ^∞ have minimizers, then the following strict inequality holds:*

$$I_{\vartheta+\kappa} < I_\vartheta + I_\kappa^\infty \tag{A.2}$$

Proof. If $\mathcal{D}$ is a minimizer for the problem I_ϑ, then $\mathcal{D}$ is a solution to the Euler equation

$$\mathcal{D} = 1_{(-\infty,\epsilon_{\mathrm{F}})}(T_{\rho_{\mathcal{D}}}) + \mathcal{D}^{(\delta)}$$

for some Fermi level $\epsilon_{\mathrm{F}} \in \mathbb{R}$. Here

$$T_{\rho_{\mathcal{D}}} = \alpha^{-1}\widetilde{T}_0 + \alpha^{-1}V + \rho_{\mathcal{D}} * |\mathbf{r}|^{-1} + g'(\rho_{\mathcal{D}}), \tag{A.3}$$

and the operator $\mathcal{D}^{(\delta)}$ satisfies $0 \leq \mathcal{D}^{(\delta)} \leq 1$ and $\mathrm{Ran}(\mathcal{D}^{(\delta)}) \subset \mathrm{Ker}(T_{\rho_{\mathcal{D}}} - \epsilon_{\mathrm{F}})$. By standard arguments, one shows that $\mathrm{spec}_{\mathrm{ess}}(T_{\rho_{\mathcal{D}}}) = [0, +\infty)$. Moreover, $T_{\rho_{\mathcal{D}}}$ is bounded from below,

$$T_{\rho_{\mathcal{D}}} \leq \alpha^{-1}\widetilde{T}_0 + V + \rho_{\mathcal{D}} * |\mathbf{r}|^{-1} \tag{A.4}$$

Since $-\sum_{k=1}^M Z_k + \int_{\mathbb{R}^3} \rho_{\mathcal{D}} = Z_{\mathrm{tot}} + 2\vartheta < -Z_{\mathrm{tot}} + 2\lambda \leq 0$, we may apply Lemma 3.2 which tells us that the operator on the right-hand side of (A.4) has infinitely many negative eigenvalues of finite multiplicity and $T_{\rho_{\mathcal{D}}}$ inherits this property. Hence, we will have $\epsilon_{\mathrm{F}} < 0$ and

$$\mathcal{D} = \sum_{n=1}^{\tilde{n}} |\phi_n\rangle\langle\phi_n| + \sum_{n=\tilde{n}+1}^{m} \nu_n |\phi_i\rangle\langle\phi_i|$$

where $\nu_n \in [0,1]$ and

$$\alpha^{-1}\widetilde{T}_0\phi_n + V\phi_n + \big(\rho_{\mathcal{D}} * \frac{1}{|\mathbf{r}|}\big)\phi_n + g'(\rho_{\mathcal{D}})\phi_n = \epsilon_n\phi_n$$

where $\epsilon_1 \leq \epsilon_2 \leq \cdots < 0$ denote the negative eigenvalues of $T_{\rho_{\mathcal{D}}}$, taking into account multiplicity. We have the following facts from [5] (requires a few additional, but easy, arguments):

(1) ϵ_1 is a nongenerate eigenvalue of $H_{\rho_{\mathcal{D}}}$;
(2) ϕ_n (and hence $\rho_{\mathcal{D}}$ belongs to $\mathbf{H}^{1/2}(\mathbb{R}^3)$;
(3) ϕ_n decays exponentially fast to zero at infinity.

Next suppose $\mathcal{D}'$ is a minimizer for the problem associated to I_κ^∞. Then

$$\widetilde{\mathcal{D}} = 1_{(-\infty,\tilde{\epsilon}_{\mathrm{F}})}(T^\infty_{\rho_{\widetilde{\mathcal{D}}}}) + \widetilde{\mathcal{D}}^{(\delta)}$$

where

$$T^\infty_{\rho_{\widetilde{\mathcal{D}}}} = \alpha^{-1}\widetilde{T}_0 + \rho_{\widetilde{\mathcal{D}}} * |\mathbf{r}|^{-1} + g'(\rho_{\widetilde{\mathcal{D}}}),$$

with $0 \leq \widetilde{\mathcal{D}} \leq 1$ and $\mathrm{Ran}(\widetilde{\mathcal{D}}) \subset \mathrm{Ker}(T^\infty_{\rho_{\widetilde{\mathcal{D}}}} - \tilde{\epsilon}_{\mathrm{F}})$ and $\tilde{\epsilon}_{\mathrm{F}} \leq 0$. Consider first the situation $\tilde{\epsilon}_{\mathrm{F}} < 0$. In this case we have that

$$\widetilde{\mathcal{D}} = \sum_{n=0}^{m} |\tilde{\phi}_n\rangle\langle\tilde{\phi}_n| + \sum_{n=m+1}^{\tilde{m}} \tilde{\nu}_n |\tilde{\phi}_n\rangle\langle\tilde{\phi}_n|$$

where every $\tilde{\phi}_n \in C^\infty(\mathbb{R}^3)$ decays exponentially to zero at infinity. By choosing $j \in \mathbb{N}$ sufficiently large, we infer that the operator

$$\mathcal{D}_j := \min\{1, \|\mathcal{D} + \mathcal{T}_{j\mathbf{e}}\widetilde{\mathcal{D}}\mathcal{T}_{-j\mathbf{e}}\|^{-1}\}\big(\mathcal{D} + \mathcal{T}_{j\mathbf{e}}\widetilde{\mathcal{D}}\mathcal{T}_{-j\mathbf{e}}\big)$$

belongs to $\mathcal{K}$ and $\mathrm{Tr}(\mathcal{D}_j) \leq (\vartheta + \kappa)$. Since both ϕ_n and $\tilde{\phi}_n$ decay exponentially to zero at infinity, a straightforward computation implies that there exists some $\delta > 0$ such that for j sufficiently large,

$$\begin{aligned}\mathcal{E}(\mathcal{D}_j) &= \mathcal{E}(\mathcal{D}) + \mathcal{E}^\infty(\widetilde{\mathcal{D}}) - \frac{2\vartheta(Z_{\mathrm{tot}} - 2\kappa)}{j} + \mathcal{O}(e^{-\delta j}) \\ &= I_\vartheta + I_\kappa^\infty - \frac{2\vartheta(Z_{\mathrm{tot}} - 2\kappa)}{j} + \mathcal{O}(e^{-\delta j})\end{aligned}$$

whence, for j large enough, (we have that $2\kappa < 2N_{\mathrm{p}} \leq Z_{\mathrm{tot}}$ for j large enough)

$$I_{\vartheta+\kappa} \leq I_{\mathrm{Tr}(\mathcal{D}_n)} \leq \mathcal{E}(\mathcal{D}_j) < I_\vartheta + I_\kappa^\infty.$$

If $\tilde{\epsilon}_{\mathrm{F}} = 0$, then zero is an eigenvalue of $T^\infty_{\rho_{\widetilde{\mathcal{D}}}}$ and there exists a L^2-normalized $\psi \in \mathrm{Ker}(T^\infty_{\rho_{\widetilde{\mathcal{D}}}}) \subset \mathbf{H}^{1/2}(\mathbb{R}^3)$ such that $\widetilde{\mathcal{D}}\psi = \beta\psi$ with $\beta > 0$. For $0 < \gamma < \beta$, both

$$\mathcal{D} + \gamma\,|\phi_{m+1}\rangle\langle\phi_{m+1}| \quad \text{and} \quad \widetilde{\mathcal{D}} - \gamma\,|\psi\rangle\langle\psi|$$

belong to $\mathcal{K}$ and a straightforward computation shows that

$$\mathcal{E}(\gamma\,|\phi_{m+1}\rangle\langle\phi_{m+1}|\,) = I_\vartheta + 2\gamma\epsilon_{m+1} + o(\gamma)$$

and

$$\mathcal{E}^\infty(\widetilde{\mathcal{D}} - \gamma\,|\psi\rangle\langle\psi|\,) = I_\kappa^\infty + o(\gamma).$$

Since

$$\mathrm{Tr}[\gamma\,|\phi_{m+1}\rangle\langle\phi_{m+1}|\,] = \vartheta + \gamma \quad \text{and} \quad \mathrm{Tr}[\widetilde{\mathcal{D}} - \gamma\,|\psi\rangle\langle\psi|\,] = \kappa - \gamma,$$

we infer that

$$I_{\vartheta+\gamma} \leq I_\vartheta + 2\gamma\epsilon_{m+1} + o(\gamma) \quad \text{and} \quad I^\infty_{\kappa-\gamma} \leq I^\infty_\kappa + o(\gamma).$$

Then, by Proposition 5.5 and for γ small enough, we conclude that

$$I_{\vartheta+\kappa} \leq I_{\vartheta+\gamma} + I^\infty_{\kappa-\gamma} \leq I_\vartheta + I^\infty_\kappa + 2\gamma\epsilon_{m+1} + o(\gamma) < I_\vartheta + I^\infty_\kappa.$$

□

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