GROUND STATE FOR THE RELATIVISTIC ONE ELECTRON ATOM

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Abstract. We study the Dirac-Maxwell system coupled with an external potential of Coulomb type. We use the Foldy–Wouthuysen (unitary) transformation of the Dirac operator and its realization as an elliptic problem in the 4-dim half space \( \mathbb{R}^4_+ \) with Neumann boundary condition. Using this approach we study the existence of a “ground state” solution.

1. Introduction and main results

The Dirac operator is a first order operator acting on the 4-spinors \( \psi : \mathbb{R}^3 \to \mathbb{C}^4 \) describing a relativistic electron given by

\[
D_0 = -i c \hbar \alpha \cdot \nabla + mc^2 \beta
\]

Here \( c \) denotes the speed of light, \( m > 0 \) the mass, \( \hbar \) the Planck’s constant, \( \alpha = (\alpha_1, \alpha_2, \alpha_3) \) and \( \beta \) are the Pauli-Dirac \( 4 \times 4 \)-matrices,

\[
\beta = \begin{pmatrix} I_2 & 0 \end{pmatrix} \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \quad k = 1, 2, 3
\]

and \( \sigma_k \) are the Pauli \( 2 \times 2 \)-matrices. We take units such that \( m = c = \hbar = 1 \).

We are interested in perturbed Dirac operators \( D_0 + \alpha_{fs} V \), \( V \) being a Coulomb potential, \( V(x) = -\frac{Z}{|x|} \), \( \alpha_{fs} = \frac{e^2 \hbar}{mc} \approx \frac{1}{137} \) is the dimensionless fine structure constant and \( Z \), positive integer, is the atomic number.

Due to the unboundedness of the spectrum of the free Dirac operator, many efforts have been devoted to the characterization and computation of the eigenvalues for the Dirac-Coulomb Hamiltonian \( D_0 + \alpha_{fs} V \), see [7] and references therein.

Here we add the interaction of the electron with its own (static) electromagnetic field. The scalar potential \( \Phi \) and the vector potential \( A = (A_1, A_2, A_3) \) of the electromagnetic field generated by the electron \( \psi \) satisfy the following (static) Maxwell equations

\[
-\Delta \Phi = 4\pi \rho; \quad -\Delta A = 4\pi J
\]

where \( \rho = |\psi|^2 \) is the charge density and \( J = (\psi, \alpha \psi) \) the current of the electron. Therefore

\[
\Phi = |\psi|^2 + \frac{1}{|x|} \quad \text{and} \quad A = (\psi, \alpha \psi) + \frac{1}{|x|}.
\]

The interaction is obtained through the minimal coupling prescription, which has, in our units, the following form

\[
D\psi = \alpha \cdot (-i \nabla - \alpha_{fs} A)\psi + \alpha_{fs} \Phi \psi + \beta \psi + \alpha_{fs} V \psi
\]

We have the following result

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Theorem 1.1. Let $V(x) = -\frac{Z}{|x|}$ with $Z \in \mathbb{N}$ the atomic number. For any $4 < Z < 124$ there exists $\mu \in (0, 1)$ and $\psi \in H^{1/2}(\mathbb{R}^3; \mathbb{C}^4) \cap \mathbb{L}^{q, \beta}(\mathbb{R}^3; \mathbb{C}^4)$ a solution of the following Maxwell-Dirac eigenvalue problem

\[
\begin{align*}
\mathbf{\alpha} \cdot (-i \nabla - \alpha A) \psi + \alpha \beta \Phi \psi + \beta \psi + \alpha A \psi &= \mu \psi \\
|\psi|_{L^2}^2 &= 1 \\
-\Delta \Phi &= 4\pi \rho = 4\pi |\psi|^2 \\
-\Delta A &= 4\pi J = 4\pi (\psi, \alpha \psi)
\end{align*}
\]

(MDC)

Moreover $(\psi, \mu)$ is (up to phase) the state of lowest positive energy of the system ("ground state").

This existence result is strictly related to the results in [9], where the Authors consider the Dirac-Fock equations for Atoms and Molecules. The equation considered in that article describe an atom (even a molecule) with a (fixed) nucleus and $N$ electrons, and takes into account the interaction of each electron with the nucleus and the other electrons, but not the interaction of the electrons with their own electric and magnetic field. Using the Hartree approximation one ends with an equation similar to the one for the atom with one electron that we consider in our model (MDC).

Let us also point out that we will prove our result via variational methods, after performing a unitary change of variables (the Foldy-Wouthuysen transformation) and a reduction of the problem to an elliptic problem in the 4-dim half space $\mathbb{R}^4_+$ with nonlinear Neumann boundary condition.

Even in this different setting, we have used in the analysis of the variational structure of the problem some ideas contained in [9] [7] [11].

2. The FW transformation and the Dirichlet to Neumann operator

Let us recall first the main properties of the free Dirac operator $D_0 = -i\mathbf{\alpha} \cdot \nabla + \beta$ (see e.g. [13]). $D_0$ is essentially self-adjoint on $C^\infty_0(\mathbb{R}^3 \setminus \{0\}; \mathbb{C}^4)$ and self-adjoint on $\mathcal{D}(D_0) = H^1(\mathbb{R}^3; \mathbb{C}^4)$. Its spectrum is purely absolutely continuous and it is given by

$$\sigma(D_0) = (-\infty, -1] \cup [1, +\infty).$$

Let define $Q_{D_0}: H^{1/2}(\mathbb{R}^3; \mathbb{C}^4) \times H^{1/2}(\mathbb{R}^3; \mathbb{C}^4) \to \mathbb{C}$ the sesquilinear form associated to the operator $D_0$.

Let denote by $\hat{u}$ or $\mathcal{F}(u)$ the Fourier transform extending the formula

$$\hat{u}(p) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{-i p \cdot x} u(x) \, dx,$$

for $u \in \mathcal{S}(\mathbb{R}^3)$.

In the (momentum) Fourier space the free Dirac operator is given by the multiplication operator $\hat{D}_0(p) = \mathcal{F} D_0 \mathcal{F}^{-1} = \mathbf{\alpha} \cdot p + \beta$ that is for each $p \in \mathbb{R}^3$ an Hermitian 4 × 4-matrix with eigenvalues

$$\lambda_1(p) = \lambda_2(p) = -\lambda_3(p) = -\lambda_4(p) = \sqrt{|p|^2 + 1} \equiv \lambda(p).$$

The unitary transformation $U(p)$ which diagonalize $\hat{D}_0(p)$ is given explicitly by

$$U(p) = a_+(p) \mathbb{1}_4 + a_-(p) \frac{\mathbf{\alpha} \cdot p}{|p|}$$

$$U^{-1}(p) = a_+(p) \mathbb{1}_4 - a_-(p) \frac{\mathbf{\alpha} \cdot p}{|p|}$$

with $a_\pm(p) = \sqrt{\frac{1}{2} (1 \pm \frac{1}{|p|^2})}$, we have

$$U(p) \hat{D}_0(p) U^{-1}(p) = \lambda(p) \beta = \sqrt{|p|^2 + 1} \beta.$$
Hence there are two orthogonal projectors \( \Lambda_\pm \) on \( L^2(\mathbb{R}^3, \mathcal{C}^4) \), both with infinite rank, given by

\[
\Lambda_\pm = \mathcal{F}^{-1}U(p)^{-1}\left(\frac{|\mu_4 + \beta|}{2}\right)U(p)\mathcal{F}.
\]

such that

\[
D_0\Lambda_\pm = \Lambda_\pm D_0 = \pm \sqrt{-\Delta + 1}\Lambda_\pm = \pm \Lambda_\pm \sqrt{-\Delta + 1}\mathbb{I}_4.
\]

The operator \( |D_0| = \sqrt{-\Delta + 1}\mathbb{I}_4 \) can be defined for all \( f \in H^1(\mathbb{R}^3, \mathcal{C}^4) \) as the inverse Fourier transform of the \( L^2 \) function \( \sqrt{|p|^2 + 1}\hat{f}(p) \) (see [10]).

Now we consider the Foldy-Wouthuysen (FW) transformation, given by the unitary transformation \( U_{FW} = \mathcal{F}^{-1}U(p)\mathcal{F} \). Under the FW transformation the projectors \( \Lambda_\pm \) become simply

\[
\Lambda_{\pm,FW} = U_{FW}\Lambda_\pm U_{FW}^{-1} = \frac{\mathbb{I}_4 + \beta}{2},
\]

and \( D_{FW} = U_{FW}D_0U_{FW}^{-1} = |D_0| \beta \) with the corresponding sesquilinear form

\[
\mathcal{Q}_{D_{FW}}(f, g) = \int_{\mathbb{R}^3} |p|^2 + 1 \left( \hat{f}(p), \beta \hat{g}(p) \right) dp = \mathcal{Q}_{D_0}(U_{FW}^{-1}f, U_{FW}^{-1}g)
\]

defined on the form domain \( H^{1/2}(\mathbb{R}^3; \mathcal{C}^4) \).

The operator \( \sqrt{-\Delta + 1} \), exactly as the fractional Laplacian, can be related to the following Dirichlet to Neumann operator (see for example [3] for problems involving the fractional Laplacian, and [4, 5] for more closely related models): given \( u \) solve the Dirichlet problem

\[
\begin{aligned}
-\partial_x^2 v - \Delta_y v + v &= 0 \quad \text{in} \quad \mathbb{R}_+^4 = \{(x, y) \in \mathbb{R} \times \mathbb{R}^3 \mid x > 0 \} \\
v(0, y) &= u(y) \quad \text{for} \quad y \in \mathbb{R}^3 = \partial\mathbb{R}_+^4.
\end{aligned}
\]

and let

\[
\mathcal{T}u(y) = \frac{\partial v}{\partial x}(0, y) = -\frac{\partial v}{\partial x}(0, y)
\]

Then \( \mathcal{T}u(y) = \mathcal{F}_y^{-1}(\sqrt{|p|^2 + 1} \hat{u}(p)) = \sqrt{-\Delta + 1} u(y) \).

Indeed, solving the equation via partial Fourier transform we get

\[
v(x, y) = \mathcal{F}_y^{-1}(\hat{u}(p))e^{-x\sqrt{|p|^2 + 1}}.
\]

In view of the FW transformation we may consider the eigenvalue problem [MDC] for the perturbed Dirac operator

\[
D_0 - \alpha_{fs}\alpha \cdot A + \alpha_{fs}\Phi + \alpha_{fs}V
\]

as follows.

Let \( (\psi_\mu, \mu) \in H^{1/2}(\mathbb{R}^3, \mathcal{C}^4) \times \mathbb{R} \) be a (weak) solution of the eigenvalue problem [MDC] and let \( \phi_\mu \) be the following extension of \( \varphi_\mu = U_{FW}\psi_\mu \) on the half-space (see lemma 3.1 below)

\[
\phi_\mu(x, y) = \mathcal{F}_y^{-1}(U(p)\hat{\psi}_\mu(p))e^{-x\sqrt{|p|^2 + 1}},
\]

then \( \phi_\mu \in H^1(\mathbb{R}_+^4, \mathcal{C}^4) \), \( (\phi_\mu)_r = \varphi_\mu \) and \( \phi_\mu \) is a (weak) solution of the following Neumann boundary value problem

\[
(P_\mu)
\begin{align*}
-\partial_x^2 \phi_\mu &- \Delta_y \phi_\mu + \phi_\mu = 0 \quad \text{in} \quad \mathbb{R}_+^4 \\
\beta \frac{\partial \phi_\mu}{\partial x} + U_{FW}(-\alpha_{fs}\alpha \cdot A + \alpha_{fs}\Phi + \alpha_{fs}V)U_{FW}^{-1}\varphi_\mu &= \mu \varphi_\mu \quad \text{on} \quad \partial\mathbb{R}_+^4 = \mathbb{R}^3 \\
|\phi_\mu|_{L^2}^2 &= 1 \\
\Phi = |U_{FW}\varphi_\mu|_{L^2}^2 + \frac{1}{2}A = (U_{FW}^{-1}\varphi_\mu, \alpha U_{FW}^{-1}\varphi_\mu) + \frac{1}{2}
\end{align*}
\]
On the other hand, if $\phi_\mu \in H^1(\mathbb{R}^4_+, \mathbb{C}^4)$ is a (weak) solution of the Neumann boundary value problem $\mathcal{P}_\mu$, setting $\varphi_\mu = (\phi_\mu)_r$, then $(U_{x_0}^{-1}\varphi_\mu, \mu) \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4) \times \mathbb{R}$ is a (weak) solution of (MDC).

3. Notation and preliminary results

To simplify the notation when clear from the context we will denote simply with $H^{1/2}$ the Sobolev space $H^{1/2}(\mathbb{R}^3, \mathbb{C}^n)$, with $H^1$ the space $H^1(\mathbb{R}^4_+, \mathbb{C}^n)$ and with $L^2$ the spaces $L^2(\mathbb{R}^3, \mathbb{C}^n)$ and $L^2(\mathbb{R}^4_+, \mathbb{C}^n)$ (where $n = 2$ or $n = 4$).

We introduce the following scalar products and norms in $H^1$, $H^{1/2}$ and $L^2$, respectively,

$$
\langle f | g \rangle_{H^1} = \int_{\mathbb{R}^4_+} ((\partial_x f, \partial_y g) + (\nabla_y f, \nabla_y g) + (f, g)), \quad \| f \|_{H^1}^2 = \langle f, f \rangle_{H^1},
$$

$$
\langle f | g \rangle_{H^{1/2}} = \int_{\mathbb{R}^3} \sqrt{|p|^2 + 1} \langle \hat{f}, \hat{g} \rangle, \quad \| f \|_{H^{1/2}}^2 = \langle f, f \rangle_{H^{1/2}},
$$

$$
|f|_{L^2}^2 = \int_{\mathbb{R}^3} |f|^2, \quad \| f \|_{L^2}^2 = \int_{\mathbb{R}^3} |f|^2
$$

where $(v, w)$ denotes the scalar product in $\mathbb{C}^n$.

The following property can be easily verified (see [4]).

**Lemma 3.1.** For $w \in H^1(\mathbb{R}^4_+)$, let $w_{tv} \in H^{1/2}(\mathbb{R}^3)$ be the trace of $w$ and define

$$
v(x, y) = \mathcal{F}^{-1}_y(\hat{w}_{tv}(p)e^{-x\sqrt{|p|^2+1}}).
$$

Then $v \in H^1(\mathbb{R}^4_+)$ and

$$
|w_{tv}|_{H^{1/2}}^2 = \| v \|_{H^1}^2 \leq \| w \|_{H^1}^2.
$$

**Remark 3.3.** We recall that for all $f \in C_0^\infty(\mathbb{R}^4)$

$$
\int_{\mathbb{R}^3} |f(0, y)|^2 dy = \int_{\mathbb{R}^3} dy \int_{+\infty}^0 \partial_x |f|^2 dx \leq 2 \| f \|_{L^2} \| \partial_x f \|_{L^2}
$$

and by density we get for all $\phi \in H^1$

$$
|\phi_{tr}|_{L^2}^2 \leq \int_{\mathbb{R}^4_+} (|\partial_x \phi|^2 + |\phi|^2) dx dy \leq \| \phi \|_{H^1}^2.
$$

**Remark 3.5.** Let us recall the following Hardy-type inequalities:

- **Hardy:** for all $\psi \in H^1(\mathbb{R}^3)$

$$
\| |x|^{-1} \psi \|_{L^2} \leq 2|\nabla \psi|_{L^2} \leq \gamma_H \| D_0 \psi \|_{L^2}
$$

where $\gamma_H = 2$.

- **Kato:** for all $\psi \in H^{1/2}(\mathbb{R}^3)$

$$
\| |x|^{-\frac{1}{2}} \psi \|_{L^2}^2 \leq \frac{\pi}{2} (-\Delta)^{1/4} \psi \|_{L^2}^2 \leq \gamma_K \| \psi \|_{H^{1/2}}^2
$$

where $\gamma_K = \frac{\pi}{2}$.

- **Tix [14]:** for all $\psi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$

$$
\| |x|^{-\frac{1}{2}} A_{\pm} \psi \|_{L^2}^2 \leq \gamma_T |A_{\pm} \psi \|_{H^{1/2}}^2
$$

where $\gamma_T = \frac{1}{2} (\frac{\pi}{2} + \frac{\pi}{2})$.

In view of the above inequalities, since $A_{\pm}$ commute with translation we have the following result.
Lemma 3.8. For any $\rho \in L^1(\mathbb{R}^3)$ and $\psi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ we have

\begin{align*}
\int_{\mathbb{R}^3} (\rho + \frac{1}{|x|})|\psi|^2(y) dy &\leq \frac{\pi}{2} |\rho|_{L^1} |(-\Delta)^{1/4}\psi|_{L^2}^2 \\
\int_{\mathbb{R}^3} (\rho + \frac{1}{|x|})|\Lambda_{\pm} \psi|^2(y) dy &\leq \gamma T |\rho|_{L^1} |\Lambda_{\pm} \psi|_{L^2}^2.
\end{align*}

Proof.

\[
\int_{\mathbb{R}^3} \left( \int_{\mathbb{R}^3} \frac{\rho(x)}{|x-y|} |\psi|^2(y) \, dx \right) dy = \int_{\mathbb{R}^3} \left( \int_{\mathbb{R}^3} \frac{|\psi|^2(y)}{|x-y|} \, dy \right) \rho(x) \, dx
\]

\[
\leq \frac{\pi}{2} |\rho|_{L^1} |(-\Delta)^{1/4}\psi|_{L^2}^2 \leq \gamma K |\rho|_{L^1} |\psi|_{H^{1/2}}^2.
\]

The second inequality can be proved in the same way since $\Lambda_{\pm}$ commute with translations.

Hence in particular for $V(x) = -\frac{Z}{|x|}$ and $Z \leq Z_c = 124$ we have that $Z\alpha_{fs}\gamma T \in (0, 1)$ and

\[
\alpha_{fs} \int |V||\Lambda_{\pm} \psi|^2 \, dy = \alpha_{fs} |V|^{1/2} \Lambda_{\pm} \psi|_{L^2}^2 \, dy \leq Z\alpha_{fs}\gamma T |\Lambda_{\pm} \psi|_{H^{1/2}}.
\]

We consider the smooth functional $I : H^1(\mathbb{R}^4_+; \mathbb{C}^4) \to \mathbb{R}$ given by

\[
I(\phi) = \|\phi_1\|_{H^1}^2 + \|\phi_2\|_{H^1}^2 + \alpha_{fs} \int_{\mathbb{R}^3} V \rho_\phi \, dy
\]

\[
+ \frac{\alpha_{fs}}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\phi(y) \rho_\phi(z)}{|y-z|} \, dy \, dz
\]

where $\phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \in H^1(\mathbb{R}^4_+; \mathbb{C}^2 \times \mathbb{C}^2)$, $\psi = U_{FW}^{-1} \phi_{tr}$, and $\rho_\phi = |\phi|^2$, $J_\phi = (\psi, \alpha \psi)$.

It is easy to check that $(\phi_{\mu, h}) \in H^1(\mathbb{R}^4_+; \mathbb{C}^4) \times \mathbb{R}$ is a weak solution of the Neumann boundary value problem $(P)$ if and only if

\[
dI(\phi_{\mu})[h] = \mu 2 \text{Re} \langle (\phi_{\mu})_{tr} | h_{tr} \rangle_{L^2} \quad \forall h \in H^1(\mathbb{R}^4_+; \mathbb{C}^4).
\]

where $dI(\phi) : H^1 \to \mathbb{R}$ is the Fréchet derivative of the functional $I$ given by

\[
dI(\phi)[h] = 2 \text{Re} \langle \phi_1 | h_1 \rangle_{H^1} - 2 \text{Re} \langle \phi_2 | h_2 \rangle_{H^1} + 2\alpha_{fs} \int_{\mathbb{R}^3} V \text{Re}(\psi, \xi) \, dy
\]

\[
+ 2\alpha_{fs} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\phi(y) \text{Re}(\phi, \xi)(z) - J_\phi(y) \cdot \text{Re}(\psi, \alpha \xi)(z)}{|y-z|} \, dy \, dz
\]

where $h = \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} \in H^1(\mathbb{R}^4_+; \mathbb{C}^2 \times \mathbb{C}^2)$ and $\xi = U_{FW}^{-1} h_{tr}$.

Let consider also $d^2I(\phi) : H^1 \times H^1 \to \mathbb{R}$, setting $\eta = U_{FW}^{-1} h_{tr}$ we have

\[
d^2I(\phi)[h; k] = 2 \text{Re} \langle k_1 | h_1 \rangle_{H^1} - 2 \text{Re} \langle k_2 | h_2 \rangle_{H^1} + 2\alpha_{fs} \int_{\mathbb{R}^3} V \text{Re}(\eta, \xi) \, dy
\]

\[
+ 2\alpha_{fs} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\phi(y) \text{Re}(\eta, \xi)(z) - J_\phi(y) \cdot \text{Re}(\psi, \alpha \xi)(z)}{|y-z|} \, dy \, dz
\]

\[
+ 4\alpha_{fs} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\text{Re}(\psi, \eta)(y) \text{Re}(\phi, \xi)(z) - \text{Re}(\psi, \alpha \eta)(y) \cdot \text{Re}(\psi, \alpha \xi)(z)}{|y-z|} \, dy \, dz
\]

Remark 3.12. Note that for any $f \in L^1 \cap L^{3/2}$ we have that (see [10, Corollary 5.10])

\[
\int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(y)f(z)}{|y-z|} = \sqrt{\frac{2}{\pi}} \int_{\mathbb{R}^3} \frac{1}{|p|^2} \langle f \rangle^2(p) \, dp \geq 0.
\]
Hence in particular

\[(3.13) \quad \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{J_\psi(y) \cdot J_\psi(z)}{|y - z|} dy \, dz \geq 0.\]

Moreover since \(|J_\psi(y)| \leq \rho_\psi(y)\) for any \(y \in \mathbb{R}^3\) and \(\psi \in H^{1/2}\), see [5, Lemma 2.1], we have that

\[(3.14) \quad \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\psi(y)\rho_\psi(z) - J_\psi(y) \cdot J_\psi(z)}{|y - z|} dy \, dz \geq 0.\]

We also recall the following convergence result. Let \(v \in H^{1/2}, f_n, g_n, h_n\) bounded sequences in \(H^{1/2}\), and one of them converge weakly to zero in \(H^{1/2}\), then we have (see for example [5, Lemma 4.1])

\[(3.15) \quad \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|f_n(y)|\, |g_n(y)| \cdot |v(z)| \cdot |h_n(z)|}{|y - z|} \, dy \, dz \rightarrow 0. \quad \text{as } n \rightarrow +\infty\]

The following lemma is essentially already contained in [6, Lemma B.1], see also [12] for related results.

**Lemma 3.16.** Let \(\chi \in C_0^\infty(\mathbb{R}^3)\), then \([\chi, U_{w1}^{-1}]\) and \([\chi, U_{w2}]\) are bounded operator from \(H^{1/2}(\mathbb{R}^3; \mathbb{C}^4) \rightarrow H^{1/2}(\mathbb{R}^3; \mathbb{C}^4)\).

Moreover, for \(R \geq 1\) let define \(\chi_{R}(y) = \chi(R^{-1}y)\). Then

\[\|\chi_{R} U_{w1}\|_{H^{1/2} \rightarrow H^{1/2}} = \|\chi_{R} U_{w2}\| = O(R^{-1}) \quad \text{as } R \rightarrow +\infty.\]

4. **Maximization problem**

Our next step will be to maximize our functional in the sets

\[\mathcal{X}_W = \{ \phi = (\phi_1, \phi_2) \in H^1(\mathbb{R}^4_+, \mathbb{C}^2 \times \mathbb{C}^2) \mid \phi_1 \in W, \ |\phi_2|_{L^2}^2 = 1 \}.\]

depending on a 1-dim vector space \(W \subset H^1(\mathbb{R}^4_+; \mathbb{C}^2)\). For each \(\phi \in \mathcal{X}_W\) we will write \(\phi_2 \in X_-\), so that \(\phi \in W \times X_-\).

Denoting \(\mathcal{G}(\phi) = |\phi_{tr}|_{L^2}^2\), the tangent space of \(\mathcal{X}_W\) at some point \(\phi \in \mathcal{X}_W\) is the set

\[T_\phi \mathcal{X}_W = \{ h \in W \times X_- \mid d\mathcal{G}(\phi)[h] \equiv 2 \Re(\phi_{tr}^* h_{tr})_{L^2} = 0 \}\]

and \(\nabla_{\mathcal{X}_W} \mathcal{I}(\phi)\), the projection of the gradient \(\nabla \mathcal{I}(\phi)\) on the tangent space \(T_\phi \mathcal{X}_W\) is given by

\[\nabla_{\mathcal{X}_W} \mathcal{I}(\phi) = \nabla \mathcal{I}(\phi) - \mu(\phi) \nabla \mathcal{G}(\phi)\]

where \(\nabla \mathcal{I}(\phi), \nabla \mathcal{G}(\phi) \in H^1\) are such that

\[\Re(\nabla \mathcal{I}(\phi)[h]_{H^1}) = d\mathcal{I}(\phi)[h] \quad \text{and} \quad \Re(\nabla \mathcal{G}(\phi)[h]_{H^1}) = d\mathcal{G}(\phi)[h]\]

for all \(h \in H^1\) and \(\mu(\phi) \in \mathbb{R}\) is such that \(\nabla_{\mathcal{X}_W} \mathcal{I}(\phi) \in T_\phi \mathcal{X}_W\).

We begin giving a result on Palais-Smale sequences for \(\mathcal{I}\) restricted on \(\mathcal{X}_W\).

**Lemma 4.1.** Fix any \(w \in H^1(\mathbb{R}^4_+; \mathbb{C}^2)\), \((w)_{tr} \neq 0\) and let \(W = \text{span}\{w\}\).

Suppose \(\phi^n \in \mathcal{X}_W\) is a Palais-Smale sequence for \(\mathcal{I}\) restricted on \(\mathcal{X}_W\), at a positive level, that is

- \(\mathcal{I}(\phi^n) = c + \epsilon_n \rightarrow c > 0\);
- \(\nabla_{\mathcal{X}_W} \mathcal{I}(\phi^n) \rightarrow 0\).

Then \(\phi^n\) is bounded and \(\|\phi^n\|_{L^2}^2 > \frac{1}{2}\).

**Proof.** We let \(\phi^* = \left(\begin{array}{c} \phi_1^* \\ \phi_2^* \end{array} \right)\). Since \(\phi_1^* \in W, W\) one dimensional, and \(0 < |(\phi_1^*)_{tr}|_{L^2}^2 \leq 1\) we have \(\|\phi_1^*\| \leq c_W\) for some constant (depending on \(W\)).
Let us denote $\psi_n = U_{FW}^{-1} \left( \phi_n^1 \right)$, $\psi^0_n = U_{FW}^{-1} \left( \phi^0_n \right)$ and $\psi_n = \psi^+_n + \psi^0_n$. In view of Remarks 3.5 and 3.12 we have, for $n$ large enough,

$$c + \epsilon_n = \mathcal{I}(\phi^n) \leq \| \phi^n_1 \|^2_{H^1} - \| \phi^n_2 \|^2_{H^1} + \alpha_{59} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\psi(y)(\rho_\psi^0 + \rho_\psi^n)(z)}{|y - z|} \, dy \, dz$$

$$\leq (1 + \alpha_{59} \gamma_T) \| \phi^n_1 \|^2_{H^1} - (1 - \alpha_{59} \gamma_T) \| \phi^n_2 \|^2_{H^1}$$

Hence we may conclude that

$$\| \phi^n_1 \|^2_{H^1} \leq c W$$,

$$\| \phi^n_2 \|^2_{H^1} \leq \frac{1 + \alpha_{59} \gamma_T}{1 - \alpha_{59} \gamma_T} \| \phi^n_1 \|^2_{H^1}$$

and also

$$\| \phi^n_1 \|^2_{H^1} + \| \phi^n_2 \|^2_{H^1} \leq \frac{2c W}{1 - \alpha_{59} \gamma_T}$$

In particular we deduce that the any Palais-Smale sequence is bounded in $H^1$.

Then we have

$$\langle \nabla_{XW} \mathcal{I}(\phi^n), \phi^n \rangle = d\mathcal{I}(\phi^n)[\phi^n] - \mu(\phi^n)2\| (\phi^n)_{tr} \|^2_{L^2}$$

$$= 2\mathcal{I}(\phi^n) - 2\mu(\phi^n)$$

$$+ \alpha_{59} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\psi(y)(\rho_\psi^0 + \rho_\psi^n)(z) - J_\psi^n(y) \cdot J_\psi^n(z)}{|y - z|} \, dy \, dz$$

and we deduce that

(4.2) \hspace{1cm} \mu(\phi^n) = c + \epsilon_n + \langle \nabla_{XW} \mathcal{I}(\phi^n), \phi^n \rangle

$$+ \frac{\alpha_{59}}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\psi(y)(\rho_\psi^0 + \rho_\psi^n)(z) - J_\psi^n(y) \cdot J_\psi^n(z)}{|y - z|} \, dy \, dz.$$

and

(4.3) \hspace{1cm} \mu(\phi^n) > 0

for $n$ large enough since the last term is nonnegative and $\langle \nabla_{XW} \mathcal{I}(\phi^n), \phi^n \rangle \to 0$.

Moreover since $\| \phi^n \|_{H^1}$ is bounded we have

$$o(1) = d\mathcal{I}(\phi^n)[\beta \phi^n] - \mu(\phi^n)2 \text{ Re}((\phi^n)_{tr})(\beta \phi^n)_{tr}_{L^2},$$

and observing that

$$\text{Re}(\psi_+(y) + \psi_-(y), \psi_+(y) - \psi_-(y)) = |\psi_+(y)|^2 - |\psi_-(y)|^2 = \rho_\psi^+(y) - \rho_\psi^-(y),$$
we deduce that
\[
\mu(\phi^a)|\psi^a|^2_{L^2} + o(1) \geq \mu(\phi^a)|\psi^a|^2_{L^2} + \frac{1}{2}dI(\phi^a)[\beta\phi^a] \\
= \mu(\phi^a)|\psi^a|^2_{L^2} + \|\phi^a\|_{H^1}^2 + \|\phi^a\|_{H^1}^2 + \alpha_{fs} \int_{\mathbb{R}^3} V\rho^a_{\psi^a} \, dy \\
- \alpha_{fs} \int_{\mathbb{R}^3} V\rho^a \, dy \\
+ \alpha_{fs} \int_{\mathbb{R}^3} \frac{\rho^a(y)(\rho^a_0 - \rho^a_0)(z)}{|y - z|} \, dxdydz \\
- \alpha_{fs} \int_{\mathbb{R}^3} \frac{J_\phi(y) \cdot (J_\phi - J_\phi^a)(z)}{|y - z|} \, dxdydz \\
\geq \mu(\phi^a)|\psi^a|^2_{L^2} + (1 - Z\alpha_{fs})\|\phi^a\|_{H^1}^2 + \|\phi^a\|_{H^1}^2 \\
- \alpha_{fs} \int_{\mathbb{R}^3} \frac{\rho^a_0}{|y - z|} \, dxdydz \\
+ \alpha_{fs} \int_{\mathbb{R}^3} \frac{\rho^a_0 - \rho^a_0}{|y - z|} \, dxdydz \\
\geq \mu(\phi^a)|\psi^a|^2_{L^2} + (1 - Z\alpha_{fs})\|\phi^a\|_{H^1}^2 + (1 - 2\alpha_{fs})\|\phi^a\|_{H^1}^2, \\
\geq \mu(\phi^a)|\psi^a|^2_{L^2},
\]
where we have used the estimate (3.10). We immediately deduce, since \(\mu(\phi^a) > 0\) for \(n\) large enough, that \(\|\psi^a_{+}\|_{L^2} > \|\psi^a_-\|_{L^2}\) which implies that \(\|\psi^a_{+}\|_{L^2} > \frac{1}{2}\). □

We now introduce the maximization problem

\[
(4.4) \quad \lambda_W = \sup_{\phi \in \mathcal{X}_W} I(\phi),
\]
and we show that \(\lambda_W\) is positive.

**Lemma 4.5.** Fix any \(w \in H^1(\mathbb{R}^4_+; \mathbb{C}^2)\) and let \(W = \text{span}\{w\}\). If \(w_{tr} \equiv 0\) then \(\sup_{\phi \in \mathcal{X}_W} I(\phi) = +\infty\); on the other hand for \(w_{tr} \neq 0\) then

\[
(4.6) \quad \sup_{\phi \in \mathcal{X}_W} I(\phi) = \lambda_W \in (0, +\infty).
\]

**Proof.** If \(w_{tr} \equiv 0\) we take a sequence \(\phi_n = \left(\frac{a_nw}{\phi_0}\right) \in \mathcal{X}_W\) with \(|a_n| \to +\infty\), for \(n \to +\infty\), and a fixed \(\phi_2 \in H^1\) such that \(|(\phi_2)_{tr}|_{L^2} = 1\). We denote \(\psi_- = U_{rw}^{-1}\left(\frac{0}{(\phi_2)_{tr}}\right)\).

Then by (3.14) we have

\[
\sup_{\phi \in \mathcal{X}_W} I(\phi) \geq I(\phi_n) \geq |a_n|^2\|w\|^2_{H^1} - \|\phi_2\|^2_{H^1} + \alpha_{fs} \int_{\mathbb{R}^3} V\rho_{\psi_-} \, dy \\
\geq |a_n|^2\|w\|^2_{H^1} - C \to +\infty \quad \text{as} \quad n \to +\infty.
\]

for some constant \(C > 0\) independent on \(n \in \mathbb{N}\).

Fix now \(w \in H^1(\mathbb{R}^4_+; \mathbb{C}^2)\) with \(|w_{tr}|_{L^2} = 1\). Denote \(W = \text{span}\{\frac{w}{\phi_0}\}\), then \(\phi = \left(\frac{\phi_1}{\phi_2}\right) \in \mathcal{X}_W\) is given by \(\phi_1 = aw\), \(a \in \mathbb{C}\) and \(|\phi_{tr}|_{L^2} = |a|^2 + |(\phi_2)_{tr}|_{L^2} = 1\).

Denote \(v_+ = U_{rw}^{-1}\left(\frac{w_0}{0}\right), \psi_+ = av_+, \psi_- = U_{rw}^{-1}\left(\frac{0}{(\phi_2)_{tr}}\right)\) and \(\psi = \psi_+ + \psi_-\).

Since \(\lambda_W = \sup_{\phi \in \mathcal{X}_W} I(\phi) \geq I\left(\frac{w}{\phi_0}\right)\), by (3.13), (3.11), (3.2) and (3.4)

\[
I\left(\frac{w}{\phi_0}\right) \geq \|w\|^2_{H^1} + \alpha_{fs} \int_{\mathbb{R}^3} V\rho_{\psi} \, dy \geq \|w\|^2_{H^1} - Z\alpha_{fs}\gamma TrU_{rw}^{-1}w_{tr}|_{H^{1/2}} \\
= \|w\|^2_{H^1} - Z\alpha_{fs}\gamma Trw_{tr}|_{H^{1/2}} \geq (1 - Z\alpha_{fs}\gamma Tr)|w|_{H^1}^2 \geq (1 - Z\alpha_{fs}\gamma Tr),
\]

hence \(\lambda_W > 0\).
Moreover, in view of (4.13), (5.11) and recalling that \( |\psi_-|_{[\mathcal{H}]^{1/2}} = |(\phi_2)_{tr}|_{[\mathcal{H}]^{1/2}} \leq \|\phi_2\|_{\mathcal{H}} \) by Lemma 3.11 and that \( |\rho_\psi|_{L^2} = |\psi|_{L^2} = |\phi_{tr}|_{L^2} = 1 \), for any \( \phi \in X_W \) we have

\[
\mathcal{I}(\phi) \leq \|\phi_1\|^2_{\mathcal{H}} - \|\phi_2\|^2_{\mathcal{H}} + \frac{\alpha_5}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_\psi(y)\rho_\psi(z)}{|y-z|} dy \, dz
\]

\[
\leq |a|^2 \|w\|^2_{\mathcal{H}} - \|\phi_2\|^2_{\mathcal{H}} + \alpha_5 \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_\psi(y)(\rho_\psi\rho_\psi)(z)}{|y-z|} dy \, dz
\]

\[
\leq |a|^2 \|w\|^2_{\mathcal{H}} - \|\phi_2\|^2_{\mathcal{H}} + \alpha_5 \gamma_T |\rho_\psi|_{L^1}(\|\psi_-\|^2_{[\mathcal{H}]^{1/2}} + |a|^2 |v_+|^2_{[\mathcal{H}]^{1/2}})
\]

\[
\leq - (1 - \alpha_6 \gamma_T) \|\phi_2\|^2_{\mathcal{H}} + C_W
\]

hence in particular \( \sup_{\phi \in X_W} \mathcal{I}(\phi) \leq C_W \) for some constant \( C_W > 0 \) depending only on \( W \).

Fix now \( w \in H^1(\mathbb{R}^3_+, \mathbb{C}^2) \) with \( |w_{tr}|_{L^2} = 1 \), to obtain additional information on the the maximization problem (4.13) we introduce the (constraint) functional \( \mathcal{J}_W : B_1 \to \mathbb{R} \) given by

\[
\mathcal{J}_W(u) = \mathcal{I} \left( \left( \frac{a(u)}{u} \right) w \right)
\]

where

\[
B_1 = \{ u \in X_- = H^1(\mathbb{R}^3_+, \mathbb{C}^2) \mid |u_{tr}|_{L^2} < 1 \}
\]

\( a(u) \) is given by the constrain equation \( |a w_{tr}|_{L^2}^2 + |u_{tr}|_{L^2}^2 = 1 \) that is \( |a|^2 = 1 - |u_{tr}|_{L^2}^2 \). By the phase invariance, without loss of generality, we can always assume that \( a(u) = \sqrt{1 - |u_{tr}|_{L^2}^2} \).

We have for any \( h \in H^1(\mathbb{R}^3_+, \mathbb{C}^2) \),

\[
d\mathcal{J}_W(u)[h] = d\mathcal{I} \left( \left( \frac{a(u)}{u} \right) w \right) \left[ \left( \frac{a(u)}{u} \right) w \right]
\]

and for \( h, k \in H^1 \)

\[
d^2 \mathcal{J}_W(u)[h; k] = Q_1[h; k] + Q_2[h; k]
\]

\[
= d\mathcal{I} \left( \left( \frac{a(u)}{u} \right) w \right) \left[ \left( \frac{d^2 a(u)}{u} \right) w \right]
\]

\[
+ d^2 \mathcal{I} \left( \left( \frac{a(u)}{u} \right) w \right) \left[ \left( \frac{da(u)}{u} \right) w \right] \left[ \left( \frac{da(u)}{u} \right) w \right]
\]

where, setting \( \eta = U_w^{-1} (0 \ u_{tr} \ 0) \), \( \xi = U_w^{-1} (0 \ h_{tr} \ 0) \), we have \( a(u) = \sqrt{1 - |\eta|^2_{L^2}} \),

\[
da(u)[h] = \frac{\text{Re}(\eta \xi)_{L^2}}{\sqrt{1 - |\eta|^2_{L^2}}} = -a(u) \frac{\text{Re}(\eta \xi)_{L^2}}{1 - |\eta|^2_{L^2}}
\]

and

\[
da^2(a(u)[h]) = -a(u) \frac{|\xi|^2_{L^2}}{1 - |\eta|^2_{L^2}} - a(u) \left( \frac{\text{Re}(\eta \xi)_{L^2}}{1 - |\eta|^2_{L^2}} \right)^2
\]
Setting \( v_+ = U_{pw}^{-1} \frac{u}{\phi} \), \( \phi = \left( \frac{a(u)}{u} \right) \) and \( \psi = U_{pw}^{-1} \phi \) we have

\[
\frac{1}{2} d J_W(u)[h] = - \text{Re}(\eta|\xi| L^2 \| w \|^2_{H^{1}} - \text{Re}(u|h)_{H^{1}} \\
- \alpha_{fs} \text{Re}(\eta|\xi| L^2 \int_{\mathbb{R}^3} V \rho_{e_+} \, dy + \alpha_{fs} \int_{\mathbb{R}^3} V \text{Re}(\eta, \xi) \, dy \\
+ \alpha_{fs} \int_{\mathbb{R}^3} V \text{Re}(a(u)v_+, \xi) \, dy - \alpha_{fs} \frac{\text{Re}(\eta|\xi| L^2 \int_{\mathbb{R}^3} V \text{Re}(a(u)v_+, \eta) \, dy}{1 - |\eta|_{L^2}^2} \\
- \alpha_{fs} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_+(y)\rho_{e_+}(z) - J_\psi(y) \cdot J_{e_+}(z)}{|y - z|} \, dy \, dz \\
+ \alpha_{fs} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_+(y)\rho_{e_+}(z) - J_\psi(y) \cdot J_{e_+}(z)}{|y - z|} \, dy \, dz \\
- \alpha_{fs} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_+(y)\rho_{e_+}(z) - J_\psi(y) \cdot J_{e_+}(z)}{|y - z|} \, dy \, dz \\
\]

It is convenient to define, for any \( \nu \in H^{1/2} \),

\[
\Gamma_\psi(\nu) = \alpha_{fs} \int_{\mathbb{R}^3} V \text{Re}(a(u)v_+, \nu) \, dy \\
+ \alpha_{fs} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_+(y)\rho_{e_+}(z) - J_\psi(y) \cdot J_{e_+}(z)}{|y - z|} \, dy \, dz \\
\]

where \( \psi = a(u)v_+ + \eta \). Remark that we have

\[
|\Gamma_\psi(\nu)| \leq C|\psi|_{H^{1/2}}|\nu|_{H^{1/2}}
\]

and

\[
\frac{1}{2} d J_W(u)[h] = - \text{Re}(\eta|\xi| L^2 \| w \|^2_{H^{1}} - \text{Re}(u|h)_{H^{1}} \\
- \alpha_{fs} \text{Re}(\eta|\xi| L^2 \int_{\mathbb{R}^3} V \rho_{e_+} \, dy + \alpha_{fs} \int_{\mathbb{R}^3} V \text{Re}(\eta, \xi) \, dy \\
- \alpha_{fs} \text{Re}(\eta|\xi| L^2 \int_{\mathbb{R}^3} \frac{\rho_+(y)\rho_{e_+}(z) - J_\psi(y) \cdot J_{e_+}(z)}{|y - z|} \, dy \, dz \\
+ \alpha_{fs} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_+(y)\rho_{e_+}(z) - J_\psi(y) \cdot J_{e_+}(z)}{|y - z|} \, dy \, dz \\
\]

In particular, for \( h = u \), that is \( \xi = \eta \), we have

\[
\frac{1}{2} d J_W(u)[u] = - |\eta|_{L^2}^2 \| w \|^2_{H^{1}} - \| u \|^2_{H^{1}} - \alpha_{fs} |\eta|_{L^2}^2 \int_{\mathbb{R}^3} V \rho_{e_+} \, dy + \alpha_{fs} \int_{\mathbb{R}^3} V \rho_\eta \, dy \\
- \alpha_{fs} |\eta|_{L^2}^2 \int_{\mathbb{R}^3} \frac{\rho_+(y)\rho_{e_+}(z) - J_\psi(y) \cdot J_{e_+}(z)}{|y - z|} \, dy \, dz \\
+ \alpha_{fs} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_+(y)\rho_{e_+}(z) - J_\psi(y) \cdot J_{e_+}(z)}{|y - z|} \, dy \, dz \\
+ \left( 1 - \frac{|\eta|_{L^2}^2}{1 - |\eta|_{L^2}^2} \right) \Gamma_\psi(\eta)
\]
hence we get
\begin{equation}
\frac{1}{2}dJ_W(u)[u] \leq -|\eta|^2_{L^2}(1 - Z\alpha_6\gamma_T)\|w\|^2_{H^1} - (1 - 2\alpha_6\gamma_T)\|u\|^2_{H^1} + \frac{1 - 2|\eta|^2_{L^2}}{1 - |\eta|^2_{L^2}}\Gamma_\psi(\eta).
\end{equation}

and in particular for all $|\eta|_{L^2} = \frac{1}{2}$ we have
\begin{equation}
\frac{1}{2}dJ_W(u)[u] \leq -|\eta|^2_{L^2}(1 - Z\alpha_6\gamma_T)\|w\|^2_{H^1} - (1 - 2\alpha_6\gamma_T)\|u\|^2_{H^1} < 0
\end{equation}

**Proposition 4.12.** Let $\{u_n\} \subset B_1 \subset H^1(\mathbb{R}^3, \mathbb{C}^2)$ be a Palais Smale sequence for $J_W$, i.e. such that $\|dJ_W(u_n)\| \to 0$ and $J_W(u_n) \to c > 0$.

Then,
(i) there exists $\kappa > 0$ such that $|\eta_n|^2_{L^2} \leq \frac{1}{2} - \kappa$ for all $n$ large enough;
(ii) $\{u_n\}$ is precompact in $H^1$.

where $\eta_n = (u_n)_{tr}$.

**Proof.** It is clear that the sequence $\phi^n = (a(u_n)w)$ is a Palais-Smale sequence for $I$ restricted to the subspace $X_W$. We can then apply Lemma 4.11 to deduce that $\{u_n\}$ is a bounded sequence in $H^1$ and $|\eta_n| < \frac{1}{2}$. We can assume that $u_n \to u$ weakly in $H^1$.

We let $v_+ = U_{pw}^{-1}(\psi_+)$, $a_n = a(u_n) \to a$ (up to subsequences) and $\psi_n = U_{pw}(\phi_n)_{tr} = a_nv_+ + \eta_n$.

(i) Suppose on the contrary that $|\eta_n|^2_{L^2} \to \frac{1}{2}$. Then from (4.10), $\Gamma_{\psi_n}(\eta_n) \leq C|\psi_n|^2_{H^1/2}|\eta_n|^2_{H^1/2}$. and the fact that $\{u_n\}$ is a bounded sequence in $H^1$, we get
\begin{align*}
\frac{1}{2}dJ_W(u_n)[u_n] &\leq -|\eta_n|^2_{L^2}(1 - Z\alpha_6\gamma_T)\|w\|^2_{H^1} - (1 - 2\alpha_6\gamma_T)\|u_n\|^2_{H^1} \\
&= -|\eta_n|^2_{L^2}(1 - Z\alpha_6\gamma_T)\|w\|^2_{H^1} + \frac{1 - 2|\eta_n|^2_{L^2}}{1 - |\eta_n|^2_{L^2}}\Gamma_\psi(\eta_n) \\
&\leq -\frac{1}{2}(1 - Z\alpha_6\gamma_T)\|w\|^2_{H^1} + o(1)
\end{align*}
a contradiction.

(ii) Since $|\eta_n|^2_{L^2} \leq \frac{1}{2} - \kappa$ and $\{u_n\}$ is a bounded sequence in $H^1$, by (4.10) we may conclude that
\[\Gamma_{\psi_n}(\eta_n) \geq -C\|dJ_W(u_n)\| = o(1)\]
for some constant $C > 0$ independent on $n$.

Now, from $u_n \to u$ weakly in $H^1$, $\eta_n \to \eta = U_{pw}^{-1}(0)_{tr}$ weakly in $H^{1/2}$ and $a_n \to a$ in $C$, since $Vv_+ \in H^{-1/2}$ we have
\[\int_{\mathbb{R}^3} V \text{Re}(a_nv_+, (\eta_n - \eta))(y) \, dy \to 0\]
and in view of equation (3.13)
\begin{align*}
\int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho_{\psi_n}(y) \text{Re}(a_nv_+, (\eta_n - \eta))(z) \frac{dy \, dz}{|y - z|} &\to 0 \\
\int_{\mathbb{R}^3 \times \mathbb{R}^3} J_{\psi_n}(y) \cdot \text{Re}(a_nv_+\alpha(\eta_n - \eta))(z) \frac{dy \, dz}{|y - z|} &\to 0
\end{align*}
then we have
\[
\frac{1}{2} dJ_W(u_n)[u_n - u] \leq \\
\leq -|\eta_n - |\eta_n|_L^2(1 - \alpha_0 \gamma_T)||u||^2_{H^1} - (1 - 2\alpha_0 \gamma_T)||u_n - u||^2_{H^1} \\
- \frac{|\eta_n - |\eta_n|_L^2 |\Gamma_{\psi_n}(\eta_n)| + o(1)}{1 - |\eta_n|_L^2} \\
\leq -|\eta_n - |\eta_n|_L^2(1 - \alpha_0 \gamma_T)||u||^2_{H^1} - (1 - 2\alpha_0 \gamma_T)||u_n - u||^2_{H^1} + o(1)
\]
Hence we may conclude that $u_n \to u$ strongly in $H^1$.

We have the following strict concavity result

**Proposition 4.13.** Let $u \in H^1$ be a critical point of $J_W$, namely $dJ_W(u)[h] = 0$ for any $h \in H^1$, such that $|u_n|_{L^2}^2 < \frac{1}{2}$.

Then $u$ is a strict local maximum for $J_W$, namely

\[
d^2J_W(u)[h; h] \leq -|h|^2_{H^1} \quad \forall h \in H^1
\]

for some $\delta > 0$.

**Proof.** Let $\phi = (\alpha(u)^w)$ and $\psi = U_{rw}^{-1} \phi_{tr} = a(u)v_+ + \eta$ where $v_+ = U_{rw}^{-1}(w_{tr})$ and $\eta = U_{rw}^{-1}(u_{tr})$. From the assumptions follows that $|\eta|_{L^2}^2 < \frac{1}{2}$.

Now, let $d^2J_W(u)[h; h] = Q_1[h; h] + Q_2[h; h]$ (see (4.10)-(4.13)). We set $\xi = U_{rw}^{-1}(0)$ and

\[
r[\xi] = \frac{\Re(\eta, \xi)_{L^2}}{1 - |\eta|_{L^2}}, \\
p[\xi; \xi] = (r[\xi])^2 \geq 0, \\
q[\xi; \xi] = \frac{\xi^2_{L^2}}{1 - |\eta|_{L^2}} + p[\xi; \xi] \geq 2p[\xi; \xi].
\]

We have $da(u)[\xi] = -a(u)r[\xi]$ and

\[
(da(u)[\xi])^2 = a(u)^2 p[\xi; \xi] \geq 0; \quad d^2a(u)[\xi; \xi] = -a(u)q[\xi; \xi] \leq 0.
\]

Since $dJ_W(u)[u] = 0$, in view of (4.10) we have $\Gamma_{\phi}(\eta) \geq 0$.

Let us compute $Q_1[h; h]$ adding a zero term for convenience, we get

\[
Q_1[h; h] = Q_1[h; h] + q[\xi; \xi]dJ_W(u)[u] = -2q[\xi; \xi]\left(||u||^2_{H^1} + \alpha_\delta \int_{R^3} V_{\rho \phi} dy \right. \\
+ \alpha_\delta \int_{R^3 \times R^3} \frac{\rho_\phi(y)\rho_{\phi}(z) - J_\phi(y) \cdot J_\phi(z)}{|y - z|} dy dz \\
- 2q[\xi; \xi]\left(||u||^2_{H^1} - \alpha_\delta \int_{R^3} V_{\rho \phi} dy \right) \\
- \alpha_\delta \int_{R^3 \times R^3} \frac{\rho_\phi(y)\rho_{\phi}(z) - J_\phi(y) \cdot J_\phi(z)}{|y - z|} dy dz \right) \\
- 2q[\xi; \xi]\frac{|\eta|_{L^2}^2}{1 - |\eta|_{L^2}} \Gamma_{\psi}(\eta)
\]

\[
\leq -2q[\xi; \xi]\left((1 - \alpha_0 \gamma_T)||u||^2_{H^1} - 2q[\xi; \xi]\left((1 - 2\alpha_0 \gamma_T)||u||^2_{H^1}
\]

Now let estimate $Q_2[h; h]$, setting $\chi = U_{rw}^{-1}(\frac{da(u)[\xi]w_{tr}}{h_{tr}}) = da(u)[\xi]v_+ + \xi$. We first note that by Hölder inequality implies

\[
\int_{R^3 \times R^3} \frac{\Re(\psi, \chi)(y) \Re(\psi, \chi)(z)}{|y - z|} dy dz \leq \int_{R^3 \times R^3} \frac{\rho_\phi(y)\rho_{\phi}(z)}{|y - z|} dy dz
\]
and by Remark 3.12 follows

\[
\int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\text{Re}(\psi, \alpha \chi)(y) \cdot \text{Re}(\psi, \alpha \chi)(z)}{|y - z|} dy \, dz \geq 0
\]

hence we have

\[
Q_2[h; \eta] \leq 2p[\xi; \xi]\|a(u)w\|_{L^2}^2 - 2\|h\|_{L^2}^2 + 2\alpha \int_{\mathbb{R}^3} V \rho_\psi(y) \, dy + 2\alpha \int_{\mathbb{R}^3} \rho_\psi(y) \rho_\chi(z) - J_\psi(y) \cdot J_\chi(z) \, dy \, dz
\]

\[
+ 4\alpha \int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho_\psi(y) \rho_\chi(z) \, dy \, dz
\]

\[
\leq 2a(u)^2 p[\xi; \xi]\|w\|_{L^2}^2 + \alpha \int_{\mathbb{R}^3} V \rho_\psi + \alpha \int_{\mathbb{R}^3} \rho_\psi(y) \rho_\chi(z) - J_\psi(y) \cdot J_\chi(z) \, dy \, dz
\]

Again it is convenient to add the following zero terms,

\[
0 = 2r[\xi] dJ(u)[h] + 2p[\xi; \xi] dJ(u)[u]
\]

\[
= -4p[\xi; \xi]\|w\|_{L^2}^2 + \alpha \int_{\mathbb{R}^3} V \rho_\psi + \alpha \int_{\mathbb{R}^3} \rho_\psi(y) \rho_\chi(z) - J_\psi(y) \cdot J_\chi(z) \, dy \, dz
\]

\[
+ 4r[\xi] \text{Re}(u|h)_{L^2} + 4r[\xi] \alpha \int_{\mathbb{R}^3} V \text{Re}(\eta, \xi) \, dy
\]

\[
+ 4r[\xi] \alpha \int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho_\psi(y) \text{Re}(\eta, \xi)(z) - J_\psi(y) \cdot \text{Re}(\eta, \alpha \xi)(z) \, dy \, dz
\]

\[
+ 4r[\xi] \Gamma_\psi(\xi) - 4p[\xi; \xi] \frac{\|\eta\|_{L^2}^2}{1 - \|\eta\|_{L^2}^2} \Gamma_\psi(\eta).
\]
In view of (4.10) \( \Gamma_\psi(\eta) \geq 0 \) and by Lemma 3.8 we have

\[
Q_2[h; h] = Q_2[h; h] + 2\rho(\|dJ_\psi(u)[h]\| + 2\rho(\|dJ_\psi(u)[h]\| + 2\rho(\|dJ_\psi(u)[h]\|)
\leq -2\rho(\|\psi\|^2_{H^1} + \alpha\int_{R^3} V \rho_{\psi + \alpha\int_{R^3} \rho_{\psi}(y) \rho_{\psi}(z) - J_\psi(y) \cdot J_\psi(z)} |y-z|)
- 2\|\psi\|^2_{H^1} + 2\alpha\int_{R^3} V \rho_{\psi} dy + 2\alpha\int_{R^3} \rho_{\psi}(y) \rho_{\psi}(z) - J_\psi(y) \cdot J_\psi(z) dydz
- 4\rho(\|\psi\|^2_{H^1} - \alpha\int_{R^3} V \rho_{\psi} dy - \alpha\int_{R^3} \rho_{\psi}(y) \rho_{\psi}(z) - J_\psi(y) \cdot J_\psi(z) dydz)
+ 4\rho(\|\psi\|^2_{H^1} - \alpha\int_{R^3} V \rho_{\psi} dy + \alpha\int_{R^3} \rho_{\psi}(y) \rho_{\psi}(z) - J_\psi(y) \cdot J_\psi(z) dydz)
\]

Therefore, since \( \rho(\|\psi\|^2_{H^1}) \geq 2\rho(\|\psi\|^2_{H^1}) \), we have

\[
Q_1[h; h] + Q_2[h; h] \leq -6(1 - Z\alpha\gamma\tau)|\psi(\|\psi\|^2_{H^1})|
- (1 - 2\alpha\gamma\tau)|\psi(\|\psi\|^2_{H^1} + 4\alpha\gamma\tau(\rho(\|\psi\|^2_{H^1} + \|\psi\|^2_{H^1} + \|\psi\|^2_{H^1}))
\]

\[
\leq -6(1 - Z\alpha\gamma\tau - 2\alpha\gamma\tau|\psi(\|\psi\|^2_{H^1} - (1 - 2\alpha\gamma\tau - 4\alpha\gamma\tau)|\psi(\|\psi\|^2_{H^1} - (1 - 2\alpha\gamma\tau - 4\alpha\gamma\tau)|\psi(\|\psi\|^2_{H^1})
\]

\[
\leq -(1 - 8\alpha\gamma\tau)|\psi(\|\psi\|^2_{H^1})|
\]

where we have used that \( \gamma\tau < \frac{1}{2}\gamma\tau, Z\alpha\gamma\tau + 2\alpha\gamma\tau = \alpha\tau(Z + 1)\gamma\tau \leq 1 \) (since \( Z \leq 123 \)).

In view of the above results we may conclude

**Proposition 4.14.** For any \( w \in H^1(R^3, C^2) \) with \( |w|_{L^2} = 1 \) there exists unique \( \phi = \phi_2(w) \), a strict global maximum of \( J_\psi \), namely

\[
J_\psi(\phi_2) = \sup_{u \in H^1} J_\psi(u) = \sup_{\phi \in \phi_2} I(\phi) = \lambda_2.
\]

Moreover

- \( dJ_\psi(\phi_2(w)) = 0 \);
- there exists \( \delta > 0 \) such that \( J_\psi(\phi_2(w))(h; h) \leq -\delta\|h\|^2 \) \( \forall h \in H^1 \);
- the map \( w \to \phi_2(w) \) is smooth and

\[
d\phi_2(w)[dP(w)] = -d_F(w, \phi_2(w))^{-1}[d_F(w, \phi_2(w))],
\]

where \( P(w) = \|w\|_{L^2} \) and

\[
F(w, h) = d_I \left( \begin{pmatrix} u(h)P(w) \\ P(w) \end{pmatrix} \right) \left[ \begin{pmatrix} d(u(h)P(w)) \\ h \end{pmatrix} \right] \) \( \forall h \in H^1 \).

**Proof.** It is clear that the equality \( \sup_{w \in B_1} J_\psi(u) = \sup_{\phi \in \phi_2} I(\phi) \) holds. The existence of a maximizer for \( J_\psi \) then follows from lemma 4.3 which shows that the supremum is strictly positive, Ekeland’s variational principle, which implies that we can find a maximizing sequence \( u_n \) which is also a Palais-Smale sequence, and Proposition 4.12 which shows that \( u_n \to u \) with \( |u_n|_{L^2} < \frac{1}{2} \).
Suppose that we have another maximizer \( \tilde{u} \). By Proposition 4.12, we deduce that 

\[ |u_{tr}|_{L^2} < \frac{1}{2}. \]

To reach a contradiction, we consider the set 

\[ \mathcal{G} = \{ g : [-1, 1] \to H^1(\mathbb{R}^4_+, \mathbb{C}^2) \mid g(-1) = u, \ g(1) = \tilde{u}, \ |(g(t))_{tr}|_{L^2} \leq \frac{1}{2} \} \]

and the min-max level 

\[ c = \sup_{u \in \mathcal{G}} \min_{t \in [-1, 1]} \mathcal{J}_W(g(t)) \]

The functional \( \mathcal{J}_W \) satisfies the Palais-Smale condition, see proposition 4.12, and the set \( B_{1/2} = \{ u \in H^1(\mathbb{R}^4_+, \mathbb{C}^2) \mid |u_{tr}|_{L^2} < 1/2 \} \) is invariant for the gradient flow generated by \( d\mathcal{J}_W \) since by \( \mathcal{J}_W(u)[u] < 0 \) on \( \partial B_{1/2} \). Then we can deduce that \( c \) is a Mountain pass critical level, and that there is a Mountain pass critical point \( \tilde{v} \) in \( B_{1/2} \), i.e. such that \( |\tilde{v}_{tr}|_{L^2} < \frac{1}{2} \), a contradiction with Proposition 4.13, since a Mountain pass critical point cannot be a strict local maximum.

Finally, to prove that the map \( w \to \phi_2(w) \) is smooth we use the implicit function theorem. Indeed let consider any open subset \( U \subset H^1 \setminus \{ w_{tr} = 0 \} \) and the smooth map \( F : U \times H^1 \to H^{-1} \) defined by 

\[ F(w, u)[h] = d\mathcal{I} \left( \left. \left( a(u) P(w) \right) \right|_{u} \right) \left[ \left( d\mathcal{J}_W(u) [h] P(w) \right) \right] \quad \forall h \in H^1. \]

Now fix \( w_0 \in U \) with \( |w_0|_{L^2} = 1 \) and let \( u_0 = \phi_2(w_0) \) and \( W_0 = \text{span}\{w_0\} \), we have 

\[ F(w_0, u_0) = d\mathcal{J}_W(u_0) = 0 \]

and the operator \( d_u F(w_0, u_0) : H^1 \to H^{-1} \) given by 

\[ (d_u F(w_0, u_0)[h][k] = d^2 \mathcal{I} \left( \left. \left( a(u_0) u_0 \right) \right|_{u_0} \right) \left[ \left( d\mathcal{J}_W(u_0) [h] u_0 \right) \right] \left( \left( d^2\mathcal{J}_W(u_0) [k] u_0 \right) \right] \]

\[ + d\mathcal{I} \left( \left. \left( a(u_0) u_0 \right) \right|_{u_0} \right) \left[ \left( d^2\mathcal{J}_W(u_0) [k] [k] \right) \right] \quad \forall h, k \in H^1 \]

is invertible. Indeed, we simply apply the Riesz theorem on Hilbert spaces (or equivalently Lax-Milgram theorem) to the symmetric, bilinear and bi-continuous, quadratic form \( Q : H^1 \times H^1 \to \mathbb{R} \) given by 

\[ Q[h, k] = -(d_u F(w_0, u_0)[h])[k]. \]

In view of Proposition 4.13, 

\[ Q[h, h] = -d^2 \mathcal{J}_W(u_0)[h, h] \geq \delta \|h\|^2 \quad \forall h \in H^1 \]

for some \( \delta > 0 \), namely \( Q \) is definite positive (coercive) and the theorem allow, hence for any \( f \in H^{-1} \) there exists unique \( h \in H^1 \) such that \( Q[h, k] = f[k] \) for any \( k \in H^1 \), namely \( d_u F(w_0, u_0)[h] = -f \).

Therefore we can apply the implicit function theorem to conclude that there exists a neighborhood \( U_0 \subset X_+ \setminus \{ w_{tr} = 0 \} \) of \( w_0 \) and a smooth map \( u : U_0 \to H^1 \) such that \( F(w, u(w)) = 0 \) for all \( w \in U_0 \).

Since we already know that for any \( w \in X_+ \setminus \{ w_{tr} = 0 \} \) there exist \( \phi_2(P(w)) \), the unique strict global maximum of \( \mathcal{J}_W \), such that \( F(w, \phi_2(P(w))) = 0 \), we may conclude that \( u(w) \equiv \phi_2(P(w)) \) for any \( w \in U_0 \).

Moreover, we have that for \( w \in U_0 \), 

\[ du(w) : H^1 \to H^1 \]

is given by 

\[ du(w)[h] = -(d_u F(w, u(w)))^{-1} [d_u F(w, u(w))[h]] \quad \forall h \in H^1. \]

\[ \square \]

**Corollary 4.15.** For any \( w \in H^1(\mathbb{R}^4_+, \mathbb{C}^2) \) with \( |w_{tr}|_{L^2} = 1 \), let \( \tilde{\phi}(w) = \left( \frac{a(\phi_2(w))}{\phi_2(w)} \right) \).

Then \( \tilde{\phi}(w) \in X_W \) is the unique (up to phase) maximizer of \( \mathcal{I} \) in \( X_W \), namely 

\[ \mathcal{I}(\tilde{\phi}(w)) = \sup_{\phi \in X_W} \mathcal{I}(\phi) = \lambda_w > 0. \]
and
\[ d\mathcal{I}(\phi(w))[h] = 2\mu(\phi(w)) \text{Re}(\langle \phi(w) \rangle_{tr}\mid h_{tr})_{L^2} \quad \forall h \in W \oplus X_- \]
where
\[ \mu(\phi(w)) = \lambda_W + \frac{\alpha_6}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho_{\psi_w}(y) \rho_{\psi_v}(z) - J_{\psi_w}(y) \cdot J_{\psi_v}(z) \frac{dydz}{|y-z|} \]
and \( \psi_w = U_{w}^{-1}(\phi(w))_{tr} \). Moreover, the following estimates hold
\begin{enumerate}[(i)]  
  \item \( \|\phi(w)\|_{H^1}^2 > \frac{1}{2} \);  
  \item \( \|\phi(w)\|_{H^1}^2 \leq \frac{1+\alpha_6\gamma T}{(1-\alpha_6\gamma T)} \lambda_W. \)
\end{enumerate}

**Proof.** We only have to show that item (ii) holds.

If \( \phi(w) \) is the maximizer for \( \mathcal{I} \) in \( X_W \), we have as in the proof of Lemma 1.1
\[ \lambda_W \leq (1 + \alpha_6\gamma T)\|\phi_1(w)\|^2_{H^1} - (1 - \alpha_6\gamma T)\|\phi_2(w)\|^2_{H^1}, \]
Moreover we have
\[ \lambda_W \geq \mathcal{I}(\phi_0) \geq \|\phi_1(w)\|^2_{H^1} + \alpha_6 \int_{\mathbb{R}^3} V \rho_{\psi_{+w}} \, dy \geq (1 - \alpha_6\gamma T)\|\phi_1(w)\|^2_{H^1}, \]
where \( \psi_{+w} = U_{w}^{-1}(\phi_0) \). Hence we may conclude that
\[ \|\phi_2(w)\|^2_{H^1} \leq \frac{\alpha_6\gamma T}{1-\alpha_6\gamma T}(1+\gamma T)\|\phi_1(w)\|^2_{H^1}, \]
and also
\[ \|\phi_1(w)\|^2_{H^1} + \|\phi_2(w)\|^2_{H^1} \leq \frac{1+\alpha_6\gamma T}{1-\alpha_6\gamma T}\|\phi_1(w)\|^2 \leq \frac{1+\alpha_6\gamma T}{(1-\alpha_6\gamma T)(1-\alpha_6\gamma T)} \lambda_W. \]

\[ \checkmark \]

**5. Proof of Theorem 1.1**

In view of the results of Proposition 4.13 it is convenient to introduce the smooth functional \( \mathcal{F} : H^1(\mathbb{R}^3_+; \mathbb{C}^2) \setminus \{w_{tr} \equiv 0\} \to \mathbb{R} \)
\[ \mathcal{F}(w) = \mathcal{I}(\phi(w)) \]
where \( \phi(w) = \left( \frac{\alpha_1(\phi(P(w))) P(w)}{\phi_2(P(w))} \right) \) and \( P(w) = \frac{w}{\|w_{tr}\|_{L^2}} \). Now in view of Proposition 4.14 we may conclude that
\[ \Lambda_1 = \inf_{w \in \mathcal{W}} \sup_{\dim \mathcal{W} = 1} \mathcal{I}(\phi(w)) = \inf_{w \in H^1(\mathbb{R}^3_+; \mathbb{C}^2)} \mathcal{I}(\phi(w)) = \inf_{w \in H^1(\mathbb{R}^3_+; \mathbb{C}^2), \{w_{tr} = 0\}} \mathcal{F}(w) \]

Let us introduce the constraint manifold \( \mathcal{W} \subset H^1(\mathbb{R}^3_+; \mathbb{C}^2) \)
\[ \mathcal{W} = \{ w \in H^1(\mathbb{R}^3_+; \mathbb{C}^2) : G(w) := \|w_{tr}\|_{L^2}^2 - 1 = 0 \} \]
and its tangent space
\[ T_w \mathcal{W} = \{ h \in H^1(\mathbb{R}^3_+; \mathbb{C}^2) : dG(w)[h] = 2 \text{Re}\langle w_{tr}\rangle_{tr} L^2 = 0 \} \]
Let us compute \( d\mathcal{F}(w)[h] = d\mathcal{I}(\phi(w))[d\phi(w)[h]]. \) For \( w \in \mathcal{W} \) and \( h \in H^1(\mathbb{R}^3_+; \mathbb{C}^2) \), we have
\[ d\phi(w)[h] = \left( \frac{d_{\phi_1(w)}(d\phi_2(w)[dP(w)[h]])}{d\phi_2(w)[dP(w)[h]]} + \frac{d_{\phi_2(w)}(dP(w)[h])}{0} \right). \]
Since
\[ 0 = d\mathcal{J}_w (\phi_2(w))[k] = d\mathcal{I}(\phi(w)) \left[ \left( \frac{d_{\phi_2(w)}[k]}{k} \right) \right] \quad \forall k \in H^1 \]
we have
\[ dF(w)[h] = dF_w(\phi_2(w))[d\phi_2(w)[dP(w)[h]]] + dI(\phi(w)) \left[ (a(\phi_2(w))dP(w)[h]) \right] \\
= a(\phi_2(w))dI(\phi(w)) \left[ (dP(w)[h]) \right]. \]
where \( dP(w)[h] = h - w \Re(w_{tr} | h_{tr})_{L^2} \) if \( w \in W \).

Since \( dF(w)[w] = 0 \) for any \( w \in W \), it is easy to see that \( W \) is indeed a natural constraint for \( F \). Hence in particular by Ekeland’s variational principle, there exists a Palais-Smale, minimizing sequence \( \{w_n\} \in W \), namely \( F(w_n) \rightarrow \Lambda_1 \) and \( \|dF(w_n)\| \rightarrow 0 \).

Now setting \( \phi_n = \phi(w_n) = (\phi_{1,n}, \phi_{2,n}) \), with \( \phi_{1,n} = a_n w_n \), \( a_n = a(\phi_2(w_n)) \), \( \phi_{2,n} = \phi_2(w_n) \) and \( \mu_n = \mu(\phi_n) \) and defining the linear continuous functional \( T_n : H^1(\R^3; \C^2) \rightarrow \R \)
\[ T_n[h] = dI(\phi_n)[(\mu_n)] - 2\mu_n \Re(a_n w_{tr} | h_{tr})_{L^2} \]
in view of Corollary 4.15 we have that \( T_n[h] = 0 \) for any \( h \in \text{span}\{w_n\} \) and \( n \in \N \).

On the other hand for any \( h \in H^1(\R^3; \C^2) \)
\[ dF(w_n)[h] = a_n dI(\phi_n) \left[ (dP(w_n)[h]) \right] = a_nT_n[dP(w_n)[h]] = a_n T_n[h] \]
and since \( \|dF(w_n)\| \rightarrow 0 \) and \( a_n > \frac{1}{2} \) we may conclude that \( T_n \rightarrow 0 \) strongly.

Since the sequence \( \{\phi_n\} \) is bounded in \( H^1(\R^3; \C^4) \) (it follows from Corollary 4.15 since \( \lambda_{w_n} \rightarrow \Lambda_1 \) we get that, up to a subsequence, \( \phi_n \rightarrow \phi \) weakly in \( H^1 \) and \( \mu_n \rightarrow \mu \), and hence,
\[ dI(\phi)[h] = 2\mu \Re(\phi_{tr}, h_{tr})_{L^2} \quad \forall h \in H^1(\R^3; \C^4). \]

(5.1) Since \( dI(\phi_n)[h] \rightarrow dI(\phi)[h] \) if \( \phi_n \rightarrow \phi \), see (3.15).

To conclude the proof of Theorem 1.1 we need to show that \( |\phi_{tr}|_{L^2} = 1 \), that is a strong convergence in \( L^2 \) of \( (\phi_{n})_{tr} \), in fact we will prove strong convergence of \( \phi_n \) in \( H^1 \).

First note that we can assume that
\[ \lim inf_{n \rightarrow \infty} d^2 F(w_n)[h; h] \geq 0 \quad \forall h \in H^1(\R^3; \C^2). \]
(5.2) This is an adaptation of of theorem 2.6 in Borwein and Preiss [2] with \( p = 2 \), \( \epsilon = \frac{1}{n} \) and \( \lambda = 1 \) (see also [1]) which states that one can find a minimizing sequence such that
\[ F(w_n) \leq \inf_{w \in W} F(w) + \frac{1}{n}, \]
\[ F(w_n) + \frac{1}{n} \Delta(w_n) \leq F(w) + \frac{1}{n} \Delta(w) \quad \text{for all } w \in W \]
where \( \Delta(y) = \sum_{k=1}^{\infty} \beta_k \|y_k - y_k\|^2_{H^1} \) for a (convergent) sequence of points \( y_k \) and reals \( \beta_k \geq 0 \) such that \( \sum_{k=1}^{\infty} \beta_k = 1 \). The above relation shows that \( w = w_n \) is a minimizer for \( G_n(w) = F(w) + \frac{1}{n} \Delta(w) \) and hence
\[ 0 \leq d^2 G_n(w_n)[h; h] = d^2 F(w_n)[h; h] + \frac{1}{n} \langle h | h \rangle_{H^1}. \]

Now with the additional information [2] on the second variations, we prove the following bound on the Lagrange multiplier \( \mu \), that it will be a key point to prove strong convergence of the minimizing sequence. We have

**Lemma 5.3.** \( \mu < 1 \)

**Proof.** Since \( w_n \) is bounded we can assume that \( w_n \rightharpoonup w \) in \( H^1 \). Take \( h \in H^1(\R^3; \C^2) \) such that \( h_{tr} \in H^1(\R^3; \C^2) \) and \( \Re(w_{tr} | h_{tr})_{L^2} = 0 \).
We set \( h_{1,n} = dP(w_n)[h] \) and \( h_{2,n} = d\phi_2(w_n)[dP(w_n)[h]] \), then we have
\[
d^2 F(w_n)[h; h] = d^2 I(\phi_n) \left[ \left( \frac{da(\phi_2, h_{2,n})}{h_{2,n}} w_n \right); \left( \frac{a_n}{h_{2,n}} \right) \right] + d^2 I(\phi_n) \left[ \left( \frac{a_n h_{1,n}}{0} \right); \left( \frac{a_n h_{1,n}}{0} \right) \right] + dI(\phi_n) \left[ \left( \frac{da(\phi_2, h_{2,n})}{h_{2,n}} h_{1,n} \right) \right] + dI(\phi_n) \left[ \left( \frac{a_n d^2 P(w_n)[h; h]}{0} \right) \right] = (I) + (II) + (III).
\]

where

\[(I) = d^2 I(\phi_n) \left[ \left( \frac{da(\phi_2, h_{2,n}) w_n}{h_{2,n}} \right); \left( \frac{a_n h_{1,n}}{0} \right) \right] + d^2 I(\phi_n) \left[ \left( \frac{a_n h_{1,n}}{0} \right); \left( \frac{a_n h_{1,n}}{0} \right) \right] \]
\[(II) = d^2 I(\phi_n) \left[ \left( \frac{a_n h_{1,n}}{0} \right); \left( \frac{a_n h_{1,n}}{0} \right) \right] \]
\[(III) = dI(\phi_n) \left[ \left( \frac{a_n d^2 P(w_n)[h; h]}{0} \right) \right].\]

In view of Proposition 4.14 for any \( w \in W \) we have for all \( h \in H^1 \)
\[
h_{2,n} = d\phi_2(w)[dP(w)[h]] = -(d_u F(w, \phi_2(w))^{-1}[d_w F(w, \phi_2(w))[h]]),
\]
where the map \( F : H^1 \setminus \{ w_{2r} = 0 \} \times H^1 \to H^{-1} \) is given by
\[
F(w, u)[k] = dI \left( \left( \frac{a(u)P(w)}{u} \right) \right) \left[ \left( \frac{da(u)k}{k} P(w) \right) \right] \quad \forall k \in H^1,
\]
let compute the operator \( d_w F(w, u) : H^1 \to H^{-1} \), for \( w \in W \) and any for \( h_1, h_2 \in H^1 \) we have
\[
(d_w F(w, u)[h_1])[h_2] = d^2 I \left( \left( \frac{a(u)w}{u} \right) \right) \left[ \left( \frac{a(u)P(w)[h_1]}{h_2} \right) \right] + dI \left( \left( \frac{a(u)w}{u} \right) \right) \left[ \left( \frac{da(u)h_2 P(w)[h_1]}{0} \right) \right].
\]

Hence we have
\[
-(d_u F(w_n, \phi_2, h_{2,n})[h_{2,n}])[h_{2,n}] = (d_w F(w_n, \phi_2, h_{2,n})[h][h_{2,n}] = (I).
\]

Recalling that
\[
(d_u F(w, u)[k])[k] = d^2 I \left( \left( \frac{a(u)w}{u} \right) \right) \left[ \left( \frac{da(u)k}{k} \right) \right] + dI \left( \left( \frac{a(u)w}{u} \right) \right) \left[ \left( \frac{a^2 u(k)k}{0} \right) \right] = d^2 J_W(u)[k; k] \quad \forall k \in H^1.
\]
in view of Proposition 4.13 we get
\[
(I) = (d_u F(w_n, \phi_2, h)[h])[h_{2,n}] = -d^2 J_W(\phi_2, h_{2,n} h_{2,n}) \geq \|h_{2,n}\|^2_{H^1}.
\]

On the other hand, we have
\[
(I) = a_n d^2 I(\phi_n) \left[ \left( \frac{a_n}{h_{1,n}} \right); \left( \frac{h_{1,n}}{0} \right) \right] - da(\phi_2, h_{2,n})[h_{2,n}]d^2 I(\phi_n) \left[ \left( \frac{a_n}{h_{2,n}} \right); \left( \frac{h_{1,n}}{0} \right) \right] + da(\phi_2, h_{2,n})[h_{2,n}] \left[ d^2 I(\phi_n) \left[ \phi_n; \left( \frac{h_{1,n}}{0} \right) \right] \right] + dI(\phi_n) \left[ \left( \frac{h_{1,n}}{0} \right) \right].
\]

Then, since \( (w_n)_{2r}[h_{1,n} L^2] = (w_n)_{2r}[dP(w_n)[h]]_{L^2} = 0 \), by Corollary 4.15 we have
\[
dI(\phi_n) \left[ \left( \frac{h_{1,n}}{0} \right) \right] = \mathcal{T}_n(h)
\]
and recalling that \( h_{1,n} = dP(w_n)[h] = h - w_n \Re((w_n)_{tr}[h]_{L^2} \to h \), as \( n \to +\infty \) strongly in \( H^1 \), we set \( \xi = U^{-1}_n(h) \), by Hölder’s and Hardy’s inequalities, we get
\[
d^2I(\phi_n) = dI(\phi_n) + 4\alpha \int_{\mathbb{R}^3} \frac{\rho_\psi(y)Re(\psi_n(z)) - J\psi_n(y) \cdot Re(\psi_n, \alpha \xi)(z)}{|y - z|} dy dz + o_n(1)
\]
\[
\leq T_n(h) + 8\alpha \int_{\mathbb{R}^3} \frac{\rho_\psi(y)|\psi_n(z)||\xi(z)}{|y - z|} dy dz + o_n(1)
\]
\[
\leq T_n(h) + C \int_{\mathbb{R}^3} \rho_\psi(y) \left( \int_{\mathbb{R}^3} \frac{|\xi(z)|^2}{|y - z|^2} dz \right)^{1/2} dy + o_n(1)
\]
\[
\leq T_n(h) + C|\nabla \xi|_{L^2} + o_n(1)
\]
and analogously, by Hölder and Hardy’s inequalities, we have
\[
d^2I(\phi_n) \leq C||h_{2,n}||_{H^1}(|\nabla \xi|_{L^2} + o_n(1))
\]
for some constant \( C > 0 \) that may change from line to line.

Hence, since \( da(\phi_n)[h_{2,n}] \leq ||h_{2,n}||_{H^1} \leq ||h_{2,n}||_{H^1} \) and \( |a_n| \leq 1 \), we get
\[
\delta ||h_{2,n}||_{L^1}^2 \leq (I) \leq C||h_{2,n}||_{H^1}(|\nabla \xi|_{L^2} + o_n(1))
\]
and we may conclude that
\[
(I) \leq C||\nabla \xi||_{L^2}^2 + o_n(1).
\]
Now, by Remark 3.12 and Hölder inequality, we have
\[
(II) \leq 2a_n^2||\nabla \xi||_{L^2}^2 + 2a_n^2 \alpha \int_{\mathbb{R}^3} V\rho_\xi dy
\]
\[
+ 8a_n^2 \alpha \int_{\mathbb{R}^3} \frac{\rho_\psi(y)\rho_\xi(z)}{|y - z|} dy dz + o_n(1)
\]
Moreover, recalling that
\[
d^2P(w_n)[h] = 3|\Re((w_n)_{tr}[h]_{L^2})|^2 w_n - 2 \Re((w_n)_{tr}[h]_{L^2} h - |h_{tr}||^2 w_n
\]
we have by Corollary 3.13
\[
(III) = \mu_n 2a_n^2 \Re((w_n)_{tr}[(d^2P(w_n)[h]_{tr})_{L^2}] + a_n T_n(d^2P(w_n)[h]_{tr})
\]
\[
= \mu_n 2a_n^2 (|\Re((w_n)_{tr}[h]_{L^2})|^2 - |h_{tr}||^2) + o_n(1)
\]
\[
= -2a_n^2 \mu_n |h_{tr}||^2 + o_n(1).
\]
Collecting the estimates above we get
\[
d^2\mathcal{F}(w_n)[h] = 2a_n^2 (||h||_{L^1}^2 - \mu_n |h_{tr}||^2_{L^2}) + 2a_n^2 \alpha \int_{\mathbb{R}^3} V\rho_\xi dy
\]
\[
+ 8a_n^2 \alpha \int_{\mathbb{R}^3} \frac{\rho_\psi(y)\rho_\xi(z)}{|y - z|} dy dz + C||\nabla \xi||_{L^2}^2 + o_n(1)
\]
Now, for fixed \( \epsilon > 0 \) we take \( h_\epsilon = e^{-\epsilon^{3/2}(|\eta||^2)} \) with \( \eta \in H^{5/2}(\mathbb{R}^3, \mathbb{C}^2) \), \( \eta(y) = \eta(|y|) \) and \( |\eta||L^2 = 1 \).

Note that
\[
||h_\epsilon||_{L^1}^2 = \frac{1}{2} e^{\epsilon^{3/2}||\eta||_{L^2}^2 + ||\eta||_{L^2}^2}
\]
and setting $\xi = U^{-1}_{FW} (\xi)_{m-n}$ we have
$$\xi(y) = e^{3/2} U^{-1}_{FW} \left( \eta(y) \right) = e^{3/2} \left( \mathcal{F}^{-1}_{\mathbb{R}^3} [a_{-}(\epsilon p y)] \right) (y)$$
hence in particular
$$\rho\xi(y) = e^3 |\mathcal{F}^{-1}_{\mathbb{R}^3} [a_{+}(\epsilon p y)]^2 (y) + e^3 |\mathcal{F}^{-1}_{\mathbb{R}^3} [a_{-}(\epsilon p y)]^2 (y)$$
where $\rho(y) = |\eta|^2 (y)$ and
$$\zeta(y) = |\mathcal{F}^{-1}_{\mathbb{R}^3} [(a_{+}(\epsilon p y) - 1)\eta]^2 (y) + |\mathcal{F}^{-1}_{\mathbb{R}^3} [a_{-}(\epsilon p y)]^2 (y) + 2 \Re(\eta, \mathcal{F}^{-1}_{\mathbb{R}^3} [(a_{+}(\epsilon p y) - 1)\eta]) (y)$$
Recalling that $a_{+}(\epsilon p y) = \sqrt{\frac{1}{2}} (1 + 1/\lambda(\epsilon p y))$, and $\lambda(p) = \sqrt{|p|^2 + 1}$, we have
$$|a_{+}(\epsilon p y) - 1| = \left| \frac{\lambda(\epsilon p y) + 1}{2\lambda(\epsilon p y)} \right| - 1 \leq \frac{1 - \lambda(\epsilon p y)}{2\lambda(\epsilon p y)} \leq \epsilon |p|^2$$
we have
$$|a_{-}(\epsilon p y)| = \left| \frac{\lambda(\epsilon p y) - 1}{2\lambda(\epsilon p y)} \right| \leq \epsilon |p|$$
(5.4)
$$|a_{-}(\epsilon p y)|_{L^2} \leq C \epsilon |p| \eta|_{L^2}$$
Therefore we get
$$d^2 \mathcal{F}(w_n)[h \varepsilon, h \varepsilon] \leq 2a^2_n (1 - \mu_n)$$
$$+ 2a^2_n \alpha_n \int \mathbb{R}^3 V(y) \rho \eta (\epsilon y) |\mathcal{F}^{-1}_{\mathbb{R}^3} [(a_{+}(\epsilon p y) - 1)\eta]^2 (y) + 8a^2_n \alpha_n \int \mathbb{R}^3 \rho \eta (\epsilon y) |\mathcal{F}^{-1}_{\mathbb{R}^3} [(a_{-}(\epsilon p y)]^2 (y) + 2 \Re(\eta, \mathcal{F}^{-1}_{\mathbb{R}^3} [(a_{+}(\epsilon p y) - 1)\eta]) (y)$$
$$+ C \epsilon |\mathcal{F}^{-1}_{\mathbb{R}^3} [a_{+}(\epsilon p y)]^2 |_{L^2} + a_n (1)$$
Here, using (3.6) we get
$$\int \mathbb{R}^3 \nabla \eta (\epsilon y) \frac{3}{2} dy = -Z \epsilon \int \mathbb{R}^3 \frac{\zeta(y)}{|y|} dy$$
$$= -Z \epsilon \int \mathbb{R}^3 \frac{|\mathcal{F}^{-1}_{\mathbb{R}^3} [(a_{+}(\epsilon p y) - 1)\eta]^2 (y)}{|y|} dy$$
$$- Z \epsilon \int \mathbb{R}^3 \frac{|\mathcal{F}^{-1}_{\mathbb{R}^3} [a_{-}(\epsilon p y)]^2 (y)}{|y|} dy$$
$$- 2Z \epsilon \int \mathbb{R}^3 \Re(\eta, \mathcal{F}^{-1}_{\mathbb{R}^3} [(a_{+}(\epsilon p y) - 1)\eta]) (y)$$
$$\leq C |\mathcal{F}^{-1}_{\mathbb{R}^3} [(a_{+}(\epsilon p y) - 1)\eta]|_{H^{1/2}} + C |\mathcal{F}^{-1}_{\mathbb{R}^3} [a_{-}(\epsilon p y)]^2 (y) + C |\mathcal{F}^{-1}_{\mathbb{R}^3} [(a_{+}(\epsilon p y) - 1)\eta]|_{H^{1/2}}$$
$$\leq C |\mathcal{F}^{-1}_{\mathbb{R}^3} [(a_{+}(\epsilon p y) - 1)\eta]|_{L^2}^2 + e^3 |\mathcal{F}^{-1}_{\mathbb{R}^3} [(a_{+}(\epsilon p y) - 1)\eta]|_{H^{1/2}}^2$$
Since for any radial function $\rho \in L^1(\mathbb{R}^3, \mathbb{R}_+)$ and for any $z \in \mathbb{R}^3$ we have
$$\int \mathbb{R}^3 \frac{\rho(y)}{|y - z|} dy \leq \int \mathbb{R}^3 \frac{\rho(y)}{|y|} dy.$$
we deduce
\[
\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_{\psi_n}(y) \rho_{\eta}(\varepsilon |z|) \varepsilon^3}{|y-z|} \, dy \, dz = \int_{\mathbb{R}^3} \rho_{\psi_n}(y) \left( \int_{\mathbb{R}^3} \frac{\rho_{\eta}(\varepsilon |z|) \varepsilon^3}{|y-z|} \, dz \right) \, dy \\
\leq \varepsilon |\rho_{\psi_n}|_{L^1} \int_{\mathbb{R}^3} \frac{\rho_{\eta}|z|}{|z|} \, dz
\]
and, by Lemma 3.8
\[
\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_{\psi_n}(y) \zeta(\varepsilon z) \varepsilon^3}{|y-z|} \, dy \, dz \leq C|\psi_n|^2_{H^{1/2}}|\zeta|_{L^1} \leq C \varepsilon^2 |\eta|_{H^2}^2 + o(\varepsilon^2)
\]
Then, by (5.2) and Lemma 3.8 we get
\[
0 \leq \lim inf_{n \to +\infty} d^2 F(w_n)[h; \hbar] \\
\leq 2a^2(1 - \mu) + 2a^2 \alpha \int_{\mathbb{R}^3} \left( -\frac{Z\varepsilon}{|y|} + \frac{4\varepsilon}{|y|} \right) \rho_{\eta}(||y||) \, dy \\
+ C \varepsilon^2 |\eta|_{H^2}^2 + o(\varepsilon^2)
\]
where \(a = \lim_n a_n\) (up to subsequence).
Hence, since \(Z > 4\) we may conclude that there exists \(\delta > 0\) and \(\varepsilon > 0\) such that
\[
0 \leq (1 - \mu) - \varepsilon \delta \int_{\mathbb{R}^3} \frac{|\eta|^2}{|y|} \, dy + C \varepsilon^2 |\eta|_{H^2}^2 \leq 1 - \mu - C\varepsilon
\]
where we have denoted with \(C\) various positive constants. \(\square\)

Now, let \(h_n = \begin{pmatrix} h_{1,n} & 0 \\ h_{2,n} & 0 \end{pmatrix} = \phi_n - \phi \to 0\) weakly in \(H^1\), define \(\xi_{+,n} = U_{F_n}^{-1}(h_{1,n})_{tr}\) and \(\xi_{-,n} = U_{F_n}^{-1}(h_{2,n})_{tr}\) and \(\xi_n = U_{F_n}(h_n)_{tr} = \xi_{+,n} + \xi_{-,n}\) we have

**Lemma 5.5.** If \(\xi_n \to 0\) weakly in \(H^{1/2}\) then
\[
\int_{\mathbb{R}^3} V \rho_{\xi_{-,n}} \, dy \to 0.
\]

**Proof.** The proof is similar, even somewhat simpler than the [Lemma B.1] \(\square\)

Then finally taking \(\xi_n = \beta h_n\). in view of Corollary 4.15 and since \(h_n = \phi_n - \phi \to 0\) by Lemma 5.5, we get
\[
o_n(1) = T_n(\xi_n) = d\mathcal{Z}(\phi_n)[\xi_n] - 2\mu_n \text{Re}(\psi_n, \xi_{+,n} - \xi_{-,n})_{L^2} \\
= 2||h_{1,n}||_{H^1}^2 + 2||h_{2,n}||_{H^1}^2 - 2\mu_n(||\xi_{+,n}||_{L^2}^2 - ||\xi_{-,n}||_{L^2}^2) \\
+ 2\alpha \int_{\mathbb{R}^3} V(\rho_{\xi_{+,n}} - \rho_{\xi_{-,n}}) \, dy \\
+ 2\alpha \int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho_{\psi_n}(y)\rho_{\xi_{+,n}}(z) - J_{\psi_n}(y) \cdot J_{\xi_{+,n}}(z) \, dy \, dz \\
- 2\alpha \int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho_{\psi_n}(y)\rho_{\xi_{-,n}}(z) - J_{\psi_n}(y) \cdot J_{\xi_{-,n}}(z) \, dy \, dz + o_n(1)
\]
since \(\mu < 1\) we may conclude that \(\phi_n \to \phi\) strongly in \(H^1\).
References

[1] L. Ambrosio and J. Feng. On a class of first order Hamilton-Jacobi equations in metric spaces. J. Differ. Equations, 256(7):2194–2245, 2014.

[2] J. M. Borwein and D. Preiss. A smooth variational principle with applications to subdifferentiability and to differentiability of convex functions. Trans. Am. Math. Soc., 303:517–527, 1987.

[3] X. Cabré and J. Solà-Morales. Layer solutions in a half-space for boundary reactions. Comm. Pure Appl. Math., 58(12):1678–1732, 2005.

[4] V. Coti Zelati and M. Nolasco. Existence of ground states for nonlinear, pseudorelativistic Schrödinger equations. Rend. Lincei Mat. Appl., 22:51–72, 2011.

[5] V. Coti Zelati and M. Nolasco. Ground states for pseudo-relativistic Hartree equations of critical type. Rev. Mat. Iberoam., 29(4):1421–1436, 2013.

[6] V. Coti Zelati and M. Nolasco. A variational approach to the Brown-Ravenhall operator for the relativistic one-electron atoms. Nonlinear Anal., Theory Methods Appl., Ser. A, Theory Methods, 136:62–83, 2016.

[7] J. Dolbeault, M. J. Esteban, and E. Séré. Variational characterization for eigenvalues of Dirac operators. Calc. Var. Partial Differential Equations, 10(4):321–347, 2000.

[8] M. J. Esteban, V. Georgiev, and E. Séré. Stationary solutions of the Maxwell-Dirac and the Klein-Gordon-Dirac equations. Calc. Var. Partial Differential Equations, 4(3):265–281, 1996.

[9] M. J. Esteban and E. Séré. Solutions of the Dirac-Fock equations for atoms and molecules. Comm. Math. Phys., 200(3):499–530, 1999.

[10] E. H. Lieb and M. Loss. Analysis. Number 14 in Graduate Studies in Mathematics. American Mathematical Society, 1997.

[11] S. Morozov and D. Müller. On the minimax principle for Coulomb-Dirac operators. Math. Z., 280(3-4):733–747, 2015.

[12] S. Morozov and S. Vugalter. Stability of atoms in the Brown-Ravenhall model. Ann. Henri Poincaré, 7(4):661–687, 2006.

[13] B. Thaller. The Dirac equation. Texts and Monographs in Physics. Springer-Verlag, Berlin, 1992.

[14] C. Tix. Strict positivity of a relativistic Hamiltonian due to Brown and Ravenhall. Bull. London Math. Soc., 30(3):283–290, 1998.

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