CONVERGENCE RATES FROM YUKAWA TO COULOMB INTERACTION IN THE THOMAS–FERMI–VON WEIZSÄCKER MODEL

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ABSTRACT. We establish uniform convergence, with explicit rate, of the solution to the Thomas–Fermi–von Weizsäcker (TFW) Yukawa model to the solution of the TFW Coulomb model, for general condensed nuclear configurations. As a consequence, we show the convergence of forces from the Yukawa to the Coulomb model. These results rely on an extension of Nazar & Ortner (2015) to the Yukawa setting. Auxiliary results of independent interest shown also include new existence, uniqueness and stability results for the Yukawa ground state.

1. INTRODUCTION

One of the challenges in molecular simulation is treating the interaction of charged particles using the Coulomb potential. Due to the long-range of the Coulomb potential $\frac{1}{|x|}$, the Yukawa potential $Y_a(x) = \frac{e^{-a|x|}}{|x|}$, for $a > 0$, is often used as a short-ranged approximation [6, 5, 15, 4, 17]. The Yukawa potential also appears in the Thomas–Fermi theory of impurity screening, where the parameter $a > 0$ represents the inverse screening length of a metal [13, 14, 1].

The aim of this paper is to establish the uniform convergence of the Yukawa ground state to the Coulomb ground state, in the Thomas–Fermi–von Weizsäcker (TFW) model. The main technical result estimates the rate of convergence. A rigorous statement is given in Theorem 3.5.

Theorem. *Let $m \in L^\infty(\mathbb{R}^3)$ represent a nuclear charge distribution satisfying*

$$m \geq 0 \qquad and \qquad \lim_{R \to \infty} \frac{1}{R} \inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m(z) \, \mathrm{d}z = +\infty.$$

Let the corresponding Coulomb ground state electron density and electrostatic potential, denoted by $u, \phi : \mathbb{R}^3 \to \mathbb{R}$, satisfy the TFW equations,

$$-\Delta u + \frac{5}{3} u^{7/3} - \phi u = 0,$$
$$-\Delta \phi = 4\pi(m - u^2),$$

and for $a > 0$, let the corresponding Yukawa ground state, denoted by (u_a, ϕ_a), satisfy the TFW Yukawa equations

$$-\Delta u_a + \frac{5}{3} u_a^{7/3} - \phi_a u_a = 0,$$
$$-\Delta \phi_a + a^2 \phi_a = 4\pi(m - u_a^2).$$

Then there exists $C > 0$ such that

$$\|u_a - u\|_{W^{2,\infty}(\mathbb{R}^3)} + \|\phi_a - \phi\|_{W^{2,\infty}(\mathbb{R}^3)} \leq Ca^2. \tag{1.1}$$

To the best of the author's knowledge, this is the first result that provides a rate of convergence for ground states from Yukawa to Coulomb interaction, for any electronic structure model.

An important consequence of (1.1) is an estimate for the rate of convergence of forces in the TFW model, when passing from the Yukawa to Coulomb interaction. Given a countable collection of nuclei $Y = (Y_j)_{j\in\mathbb{N}} \subset \mathbb{R}^3$ and $a > 0$, the TFW Yukawa and Coulomb energy densities, $\mathcal{E}_a(Y;x)$ and $\mathcal{E}(Y;x)$ respectively, can be defined. It follows from (1.1) that

$$\left| \int_{\mathbb{R}^3} \left(\frac{\partial \mathcal{E}_a}{\partial Y_k} - \frac{\partial \mathcal{E}}{\partial Y_k} \right)(Y;x) \, \mathrm{d}x \right| \le Ca^2. \tag{1.2}$$

A rigorous statement of this result is given in Theorem 4.1.

In a forthcoming article [7], the aim will be to generalise the analysis of variational problems for the mechanical response to defects in an infinite crystal [8] to electronic structure models, using the TFW model with Coulomb interaction. The uniform convergence of forces from Yukawa to Coulomb suggests that one could construct an approximate mechanical response problem using the Yukawa interaction. This could be more efficient for the purposes of numerical simulations as it replaces the long-range Coulomb interaction with the short-ranged Yukawa interaction. The result (1.2) suggests that the error in the electron density may propagate into an $O(a^2)$ error in the equilibrium configuration. This will be explained in future work.

The remainder of this article is organised as follows: In Section 2 the definition of the TFW model is recalled and the relevant existing results are summarised. In Section 3 the main technical results are stated, including the rigorous statement of the convergence result (1.1). Applications are presented in Section 4, followed by the detailed proofs of the results in Section 5. An additional technical argument is given in the Appendix, that extends uniqueness of the Yukawa ground state to all $a > 0$.

Remark 1. The analytical approach presented closely follows and adapts the study of the TFW equations in [6, 11]. An overview of the TFW equations can be found in [11] and [17] provides a background on the Yukawa potential and its various applications.

To the best of the author's knowledge, the closest existing result to (1.1) in the literature is [6, Proposition 2.30], which shows $u_a \to u$ strongly in $H^1_{\mathrm{loc}}(\mathbb{R}^3)$ as $a \to 0$, for periodic and neutral TFW systems, but does not estimate the rate. □

2. The TFW Yukawa Model

For $p \in [1, \infty]$ define the function spaces

$$L^p_{\mathrm{loc}}(\mathbb{R}^3) := \{ f : \mathbb{R}^3 \to \mathbb{R} \mid \forall K \subset \mathbb{R}^3 \text{ compact}, f \in L^p(K) \} \quad \text{and}$$

$$L^p_{\mathrm{unif}}(\mathbb{R}^3) := \{ f \in L^p_{\mathrm{loc}}(\mathbb{R}^3) \mid \sup_{x\in\mathbb{R}^3} \|f\|_{L^p(B_1(x))} < \infty \}.$$

For $k \in \mathbb{N}$, $H^k_{\mathrm{loc}}(\mathbb{R}^3), H^k_{\mathrm{unif}}(\mathbb{R}^3)$ are defined analogously. For a multi-index $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, define the partial derivative $\partial^\alpha = \partial_1^{\alpha_1}\partial_2^{\alpha_2}\partial_3^{\alpha_3}$. Throughout this paper, α, β denote three-dimensional multi-indices.

The Coulomb interaction, for $f, g \in L^{6/5}(\mathbb{R}^3)$, is given by

$$D_0(f,g) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{f(x)g(y)}{|x-y|} \, \mathrm{d}x \, \mathrm{d}y = \int_{\mathbb{R}^3} \left(f * \tfrac{1}{|\cdot|} \right)(y)g(y) \, \mathrm{d}y.$$

and is finite due to the Hardy–Littlewood–Sobolev estimate [2]. The Yukawa interaction is a short-range approximation to the Coulomb interaction, with the Yukawa potential $Y_a(x) = \frac{e^{-a|x|}}{|x|}$, for $a > 0$, replacing the Coulomb potential $\frac{1}{|x|}$. The parameter $a > 0$ controls the range of the interaction, in particular one formally recovers the long-ranged Coulomb interaction as $a \to 0$. The Yukawa interaction, for $a > 0$ and $f, g \in L^2(\mathbb{R}^3)$, is given by

$$D_a(f, g) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{f(x)e^{-a|x-y|}g(y)}{|x-y|} \, \mathrm{d}x \, \mathrm{d}y = \int_{\mathbb{R}^3} (f * Y_a)(y)g(y) \, \mathrm{d}y,$$

which is finite as Cauchy-Schwarz' and Young's inequality for convolutions imply

$$|D_a(f, g)| \le \|Y_a\|_{L^1(\mathbb{R}^3)}\|f\|_{L^2(\mathbb{R}^3)}\|g\|_{L^2(\mathbb{R}^3)} \le Ca^{-2}\|f\|_{L^2(\mathbb{R}^3)}\|g\|_{L^2(\mathbb{R}^3)}.$$

Let $a > 0$ and $m \in L^2(\mathbb{R}^3), m \ge 0$, denote the charge density of a finite nuclear cluster, then the corresponding TFW Yukawa energy functional is defined, for $v \in H^1(\mathbb{R}^3)$, by

$$E_a^{\mathrm{TFW}}(v, m) = C_{\mathrm{W}} \int_{\mathbb{R}^3} |\nabla v|^2 + C_{\mathrm{TF}} \int_{\mathbb{R}^3} v^{10/3} + \frac{1}{2}D_a(m - v^2, m - v^2). \tag{2.1}$$

The function v corresponds to the positive square root of the electron density. The first two terms of (2.1) model the kinetic energy of the electrons while the third term models the Coulomb energy. This definition of the Coulomb energy is only valid for smeared nuclei. The energy (2.1) can be rescaled to ensure that $C_{\mathrm{W}} = C_{\mathrm{TF}} = 1$.

To construct the electronic ground state for an infinite arrangement of nuclei (e.g., crystals), it is necessary to restrict admissible nuclear charge densities to $m \in L^1_{\mathrm{unif}}(\mathbb{R}^3), m \ge 0$, satisfying

$$(\mathrm{H1}) \quad \sup_{x \in \mathbb{R}^3} \int_{B_1(x)} m(z) \, \mathrm{d}z < \infty,$$

$$(\mathrm{H2}) \quad \lim_{R \to \infty} \inf_{x \in \mathbb{R}^3} \frac{1}{R} \int_{B_R(x)} m(z) \, \mathrm{d}z = \infty.$$

The property (H1) guarantees that no clustering of infinitely many nuclei occurs at any point in space whereas (H2) ensures that there are no large regions that are devoid of nuclei.

For each m satisfying (H1)–(H2), [11, Theorem 6.10] guarantees the existence and uniqueness of a ground state (u, ϕ) satisfying

$$-\Delta u + \frac{5}{3}u^{7/3} - \phi u = 0, \tag{2.2a}$$

$$-\Delta \phi = 4\pi(m - u^2), \tag{2.2b}$$

Similarly, as remarked in [6, Chapter 6], it also follows that for sufficiently small $a > 0$, the existence and uniqueness of the Yukawa ground state (u_a, ϕ_a), solving

$$-\Delta u_a + \frac{5}{3}u_a^{7/3} - \phi_a u_a = 0, \tag{2.3a}$$

$$-\Delta \phi_a + a^2 \phi_a = 4\pi(m - u_a^2), \tag{2.3b}$$

The equation (2.2b) arises from the Coulomb interaction, as $\frac{1}{4\pi|\cdot|}$ is the Green's function for the Laplacian on $\mathbb{R}^3$, while (2.3b) is obtained for the Yukawa problem, as $\frac{1}{4\pi}Y_a$ is the Green's function for $-\Delta + a^2$ on $\mathbb{R}^3$, $a > 0$.

Definition 1. *In this article, for any nuclear configuration m satisfying* (H1)–(H2), *the ground state corresponding to m refers to the unique solution* (u, ϕ) *to* (2.2). *For* $a > 0$, *the Yukawa ground state corresponding to m refers to the unique solution* (u_a, ϕ_a) *to* (2.3). □

3. Main Results

3.1. **Regularity estimates.** This section generalises the TFW pointwise stability estimate and its consequences [11] from the Coulomb to the Yukawa setting.

The proofs of the main results in the next section require uniform regularity estimates for Yukawa systems refining those shown in [6], provided that $a \in (0, a_0]$ for some $a_0 > 0$.

The main regularity estimate (3.1) relies on uniform variants of (H1)–(H2), so the class of nuclear configurations $\mathcal{M}_{L^2}$, defined in [11], is used. Given $M, \omega_0, \omega_1 > 0$, let $\omega = (\omega_0, \omega_1)$ and define

$$\mathcal{M}_{L^2}(M, \omega) = \left\{ m \in L^2_{\mathrm{unif}}(\mathbb{R}^3) \; \middle| \; \|m\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M, \right.$$
$$\left. \forall R > 0 \; \inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m(z) \, \mathrm{d}z \geq \omega_0 R^3 - \omega_1 \right\}. \quad (3.1)$$

As each nuclear distribution $m \in \mathcal{M}_{L^2}(M, \omega)$ satisfies (H1)–(H2), [6, Chapter 6] guarantees the existence of corresponding ground states (u_a, ϕ_a) for sufficiently small a. The proof of [6, Proposition 2.2, Chapter 6] is adapted to extend existence and uniqueness of Yukawa ground states to all $a > 0$. In addition, the uniformity in upper and lower bounds on $m \in \mathcal{M}_{L^2}(M, \omega)$ yields regularity estimates and lower bounds on these ground states which are also uniform.

Proposition 3.1. *Let* $a_0 > 0$ *and* $m \in \mathcal{M}_{L^2}(M, \omega)$, *then for any* $0 < a \leq a_0$ *there exists* (u_a, ϕ_a) *solving* (2.3), *satisfying* $u_a \geq 0$ *and*

$$\|u_a\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_a\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(a_0, M), \quad (3.2)$$

where the constant $C(a_0, M)$ *is increasing in both* a_0 *and* M.

Proposition 3.1 can be generalised to obtain existence of Yukawa ground states corresponding to finite nuclear configurations, for sufficiently small $a > 0$. The following result will be used in Proposition 4.2 to compare the Yukawa ground state with its finite approximation.

Proposition 3.2. *For any nuclear distribution* $m : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$, *satisfying*

$$\|m\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M,$$

there exists $a_0 = a_0(m) > 0$ *such that for all* $0 < a \leq a_0$, *there exists* (u_a, ϕ_a) *solving* (2.3), *satisfying* $u_a \geq 0$ *and*

$$\|u_a\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_a\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M). \quad (3.3)$$

If $\int_{B_{R_0}(x)} m \geq c_0 > 0$ *for some* $x \in \mathbb{R}^3$ *and* R_0, c_0, *then* $a_0 = a_0(R_0, c_0) > 0$.

Proposition 3.3. *Let* $a_0 > 0$ *and* $m \in \mathcal{M}_{L^2}(M, \omega)$, *then for all* $0 < a \leq a_0$ *the corresponding Yukawa ground state* (u_a, ϕ_a) *is unique and there exists* $c_{a_0, M, \omega} > 0$ *such that the electron density* u_a *satisfies*

$$\inf_{x \in \mathbb{R}^3} u_a(x) \geq c_{a_0, M, \omega} > 0. \quad (3.4)$$

Assuming higher regularity of the nuclear distributions implies higher regularity of the ground state. Therefore define for $k \in \mathbb{N}_0$

$$\mathcal{M}_{H^k}(M, \omega) = \left\{ m \in H^k_{\text{unif}}(\mathbb{R}^3) \;\middle|\; \|m\|_{H^k_{\text{unif}}(\mathbb{R}^3)} \leq M, \right.$$

$$\left. \forall\, R > 0 \; \inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m(z)\, \mathrm{d}z \geq \omega_0 R^3 - \omega_1 \right\}.$$

Arguing by induction and applying the uniform lower bound (3.4) yields the following result.

Corollary 3.4. *Let $a_0 > 0$, $k \in \mathbb{N}_0$ and $m \in \mathcal{M}_{H^k}(M, \omega)$, then for all $0 < a \leq a_0$ the corresponding Yukawa ground state (u_a, ϕ_a) satisfies*

$$\|u_a\|_{H^{k+4}_{\text{unif}}(\mathbb{R}^3)} + \|\phi_a\|_{H^{k+2}_{\text{unif}}(\mathbb{R}^3)} \leq C(a_0, k, M, \omega). \tag{3.5}$$

3.2. **Uniform Yukawa estimates.** The main result of this article is a uniform estimate comparing the Yukawa and Coulomb ground states corresponding to the same nuclear configuration. This result is essentially a consequence of [11, Theorems 3.4 and 3.5].

In the following, $(u, \phi) = (u_0, \phi_0)$ denotes the corresponding Coulomb ground state solving (2.2), i.e the ground state with Yukawa parameter $a = 0$.

Theorem 3.5. *Suppose $a_0 > 0$, $k \in \mathbb{N}_0$, $m \in \mathcal{M}_{H^k}(M, \omega)$ and let (u, ϕ) denote the corresponding Coulomb ground state. For $0 < a \leq a_0$, let (u_a, ϕ_a) denote the corresponding Yukawa ground state, then there exists $C = C(a_0, k, M, \omega) > 0$ such that*

$$\|u_a - u\|_{W^{k+2,\infty}(\mathbb{R}^3)} + \|\phi_a - \phi\|_{W^{k+2,\infty}(\mathbb{R}^3)} \leq C a^2. \tag{3.6}$$

Remark 2. The error term in (3.6) arises from the additional term in the Yukawa equation (2.3b), as opposed to due to a difference in nuclear distributions in [11, Theorems 3.4 and 3.5]. For this reason, the author believes that an analogous result to Theorem 3.5 also holds for point charge nuclei. $\qquad\square$

Theorem 3.5 can be generalised to compare two Yukawa ground states (u_{a_1}, ϕ_{a_1}), (u_{a_2}, ϕ_{a_2}) corresponding to the same nuclear configuration, where the parameters a_1, a_2 differ.

Corollary 3.6. *Let $a_0 > 0$, $k \in \mathbb{N}_0$, $m \in \mathcal{M}_{H^k}(M, \omega)$ and suppose $0 < a_1 \leq a_2 \leq a_0$, then let $(u_{a_1}, \phi_{a_1}), (u_{a_2}, \phi_{a_2})$ denote the corresponding Yukawa ground states. There exists $C = C(a_0, k, M, \omega) > 0$ such that*

$$\|u_{a_1} - u_{a_2}\|_{W^{k+2,\infty}(\mathbb{R}^3)} + \|\phi_{a_1} - \phi_{a_2}\|_{W^{k+2,\infty}(\mathbb{R}^3)} \leq C \left(a_2^2 - a_1^2 \right). \tag{3.7}$$

3.3. **Pointwise Yukawa estimates.** Theorems 3.7 and 3.8 extend [11, Theorems 3.4 and 3.5] to the Yukawa model and require the class of test functions

$$H_\gamma = \left\{ \xi \in H^1(\mathbb{R}^3) \;\middle|\; |\nabla \xi(x)| \leq \gamma |\xi(x)| \,\forall\, x \in \mathbb{R}^3 \right\} \tag{3.8}$$

for some $\gamma > 0$. Observe that $e^{-\widetilde{\gamma}|\cdot|} \in H_\gamma$ for any $0 < \widetilde{\gamma} \leq \gamma$.

Theorem 3.7. *Let $m_1 \in \mathcal{M}_{L^2}(M, \omega)$, and let $m_2 : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ satisfy*

$$\|m_2\|_{L^2_{\text{unif}}(\mathbb{R}^3)} \leq M',$$

then there exists $a_1 = a_1(\omega, m_2) > 0$ such that for all $0 < a \leq a_1$ there exist solutions $(u_{1,a}, \phi_{1,a})$ and $(u_{2,a}, \phi_{2,a})$ to (2.3) corresponding to m_1, m_2, where $(u_{2,a}, \phi_{2,a})$ satisfies $u_{2,a} \geq 0$ and

$$\|u_{2,a}\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_{2,a}\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M'), \tag{3.9}$$

independently of a. Define

$$w = u_{1,a} - u_{2,a}, \quad \psi = \phi_{1,a} - \phi_{2,a}, \quad R_m = 4\pi(m_1 - m_2),$$

then there exist $C = C(M, M', \omega), \gamma = \gamma(M, M', \omega) > 0$, such that for any $\xi \in H_\gamma$

$$\int_{\mathbb{R}^3} \left(\sum_{|\alpha_1| \leq 4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \leq 2} |\partial^{\alpha_2} \psi|^2 \right) \xi^2 \leq C \int_{\mathbb{R}^3} R_m \xi^2. \tag{3.10}$$

In particular, for any $y \in \mathbb{R}^3$,

$$\sum_{|\alpha| \leq 2} |\partial^\alpha w(y)|^2 + |\psi(y)|^2 \leq C \int_{\mathbb{R}^3} |R_m(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x. \tag{3.11}$$

Theorem 3.7 can be generalised to obtain higher-order pointwise estimates, but this requires that $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$ for some $k \in \mathbb{N}_0$ to ensure that *both* $\inf u_1, \inf u_2 > 0$.

Theorem 3.8. *Let $a_0 > 0$, $k \in \mathbb{N}_0$, $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$ and for $0 < a \leq a_0$, let $(u_{1,a}, \phi_{1,a}), (u_{2,a}, \phi_{2,a})$ denote the corresponding Yukawa ground states. Define*

$$w = u_{1,a} - u_{2,a}, \quad \psi = \phi_{1,a} - \phi_{2,a}, \quad R_m = 4\pi(m_1 - m_2),$$

then there exist $C = C(a_0, k, M, \omega), \gamma = \gamma(a_0, M, \omega) > 0$, independent of a, such that for any $\xi \in H_\gamma$

$$\int_{\mathbb{R}^3} \left(\sum_{|\alpha_1| \leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \leq k+2} |\partial^{\alpha_2} \psi|^2 \right) \xi^2 \leq C \int_{\mathbb{R}^3} \sum_{|\beta| \leq k} |\partial^\beta R_m|^2 \xi^2. \tag{3.12}$$

In particular, for any $y \in \mathbb{R}^3$,

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(y)|^2 \leq C \int_{\mathbb{R}^3} \sum_{|\beta| \leq k} |\partial^\beta R_m(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x. \tag{3.13}$$

4. APPLICATIONS

4.1. Yukawa and Coulomb forces.
Let $\eta \in C^\infty_{\mathrm{c}}(B_{R_0}(0))$ be radially symmetric and satisfy $\eta \geq 0$ and $\int_{\mathbb{R}^3} \eta = 1$ describe the charge density of a single (smeared) nucleus, for some fixed $R_0 > 0$. For any countable collection of nuclear coordinates $Y = (Y_j)_{j \in \mathbb{N}} \in (\mathbb{R}^3)^{\mathbb{N}}$, let the corresponding nuclear configuration be defined by

$$m_Y(x) = \sum_{j \in \mathbb{N}} \eta(x - Y_j). \tag{4.1}$$

A natural space of nuclear coordinates, related to the $\mathcal{M}_{H^k}$ spaces is

$$\mathcal{Y}_{L^2}(M, \omega) := \{ Y \in (\mathbb{R}^3)^{\mathbb{N}} \mid m_Y \in \mathcal{M}_{L^2}(M, \omega) \}. \tag{4.2}$$

For any $Y \in \mathcal{Y}_{L^2}(M, \omega)$ and $a > 0$, there exists a unique Yukawa ground state (u_a, ϕ_a) corresponding to $m = m_Y$. Two definitions for the energy density for an infinite system

are provided, for bounded $\Omega \subset \mathbb{R}^3$:

$$\int_\Omega \mathcal{E}_{1,a}(Y;x) \, \mathrm{d}x := \int_\Omega |\nabla u_a|^2 + \int_\Omega u_a^{10/3} + \frac{1}{2} \int_\Omega \phi_a(m - u_a^2), \tag{4.3}$$

$$\int_\Omega \mathcal{E}_{2,a}(Y;x) \, \mathrm{d}x := \int_\Omega |\nabla u_a|^2 + \int_\Omega u_a^{10/3} + \frac{1}{8\pi} \left(\int_\Omega |\nabla \phi_a|^2 + a^2 \int_\Omega \phi_a^2 \right), \tag{4.4}$$

which satisfy $\mathcal{E}_{1,a}(Y;\cdot), \mathcal{E}_{2,a}(Y;\cdot) \in L^1_{\text{unif}}(\mathbb{R}^3)$.

Suppose now that $\Omega \subset \mathbb{R}^3$ is a charge-neutral volume [20], that is, if n is the unit normal to $\partial\Omega$, then $\nabla\phi_a \cdot n = 0$ on $\partial\Omega$. Recall (2.3b),

$$-\Delta\phi_a + a^2\phi_a = 4\pi(m - u_a^2),$$

it then follows that

$$\frac{1}{8\pi} \left(\int_\Omega |\nabla\phi_a|^2 + a^2 \int_\Omega \phi_a^2 \right) = \frac{1}{8\pi} \int_\Omega (-\Delta\phi_a + a^2\phi_a)\phi_a + \int_{\partial\Omega} \phi_a\nabla\phi_a \cdot n = \frac{1}{2} \int_\Omega \phi_a(m - u_a^2),$$

hence

$$\int_\Omega \mathcal{E}_{1,a}(Y;x) \, \mathrm{d}x = \int_\Omega \mathcal{E}_{2,a}(Y;x) \, \mathrm{d}x.$$

Similarly, for finite systems and $\Omega = \mathbb{R}^3$, the two energies (4.3)–(4.4) agree. Thus $\mathcal{E}_{1,a}, \mathcal{E}_{2,a}$ are two energy densities which are well-defined for infinite configurations.

Given $Y \in \mathcal{Y}_{L^2}(M, \omega)$, similarly define the Coulomb energy densities $\mathcal{E}_1(Y;\cdot), \mathcal{E}_2(Y;\cdot) \in L^1_{\text{unif}}(\mathbb{R}^3)$ [11]

$$\mathcal{E}_1(Y;\cdot) := |\nabla u|^2 + u^{10/3} + \frac{1}{2}\phi(m - u^2), \tag{4.5}$$

$$\mathcal{E}_2(Y;\cdot) := |\nabla u|^2 + u^{10/3} + \frac{1}{8\pi}|\nabla\phi|^2. \tag{4.6}$$

By comparing the Yukawa and Coulomb energy densities, (4.3)–(4.4) with (4.5)–(4.6) respectively, then applying Theorem 3.5 and Proposition 3.2 yields the convergence of the energy densities: for all $0 < a \le a_0$

$$\|\mathcal{E}_{1,a} - \mathcal{E}_1\|_{L^2_{\text{unif}}(\mathbb{R}^3)} + \|\mathcal{E}_{2,a} - \mathcal{E}_2\|_{H^1_{\text{unif}}(\mathbb{R}^3)} \le C(a_0, M)a^2. \tag{4.7}$$

In (4.7), the regularity of the difference $\mathcal{E}_{1,a} - \mathcal{E}_1$ is limited by the nuclear distribution $m \in L^2_{\text{unif}}(\mathbb{R}^3)$, whereas this term does not appear in $\mathcal{E}_{2,a} - \mathcal{E}_2$, hence the latter possesses additional regularity.

The next result shows that the force generated by a nucleus converges when passing from the Yukawa to the Coulomb model.

Theorem 4.1. *Let $a_0 > 0$, $Y \in \mathcal{Y}_{L^2}(M, \omega)$ and $i \in \{1, 2\}$, then for all $0 < a \le a_0$ and $k \in \mathbb{N}$, the Yukawa force density $\partial_{Y_k}\mathcal{E}_{i,a}(Y, \cdot) \in L^1(\mathbb{R}^3)$ exists and satisfies*

$$\int_{\mathbb{R}^3} \frac{\partial\mathcal{E}_{1,a}}{\partial Y_k}(Y;x) \, \mathrm{d}x = \int_{\mathbb{R}^3} \frac{\partial\mathcal{E}_{2,a}}{\partial Y_k}(Y;x) \, \mathrm{d}x = \int_{\mathbb{R}^3} \phi_a(x) \frac{\partial m_Y(x)}{\partial Y_k} \, \mathrm{d}x. \tag{4.8}$$

In addition, the Coulomb force density $\partial_{Y_k}\mathcal{E}_i(Y, \cdot) \in L^1(\mathbb{R}^3)$ also exists and there exists $C = C(a_0, M, \omega) > 0$ such that for all $0 < a \le a_0$

$$\left| \int_{\mathbb{R}^3} \left(\frac{\partial\mathcal{E}_{i,a}}{\partial Y_k} - \frac{\partial\mathcal{E}_i}{\partial Y_k} \right)(Y;x) \, \mathrm{d}x \right| \le Ca^2. \tag{4.9}$$

The expression (4.8) shows that the forces generated by the energy densities $\mathcal{E}_{1,a}$ and $\mathcal{E}_{2,a}$ are identical. Also, (4.9) establishes an $O(a^2)$ convergence of forces when passing from the Yukawa to the Coulomb model.

4.2. **Thermodynamic limit estimates.** The following result extends [11, Proposition 4.1] to the Yukawa setting, providing an estimate for comparing the infinite Yukawa ground state with its finite approximation, over compact sets, thus providing explicit rates of convergence for the thermodynamic limit. This is discussed in Remark 3.

Interpreted differently, the result yields estimates on the decay of the perturbation from the bulk electronic structure at a domain boundary.

Proposition 4.2. *Let $m \in \mathcal{M}_{L^2}(M, \omega)$, $\Omega \subset \mathbb{R}^3$ be open and suppose there exists $m_\Omega : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ such that $m_\Omega = m$ on Ω and $\|m_\Omega\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M$ (e.g., $m_\Omega = m\chi_\Omega$). Then there exists $a_0 = a_0(\omega, m_\Omega) > 0$ such that for all $0 < a \leq a_0$ there exists a ground state (u_a, ϕ_a) corresponding to m and $(u_{\Omega,a}, \phi_{\Omega,a})$ solving (2.3) with $m = m_\Omega$, $u_{\Omega,a} \geq 0$ and $C = C(a_0, M, \omega), \gamma = \gamma(a_0, M, \omega) > 0$, independent of a and Ω, such that for all $y \in \Omega$*

$$\sum_{|\alpha| \leq 2} |\partial^\alpha (u_a - u_{\Omega,a})(y)| + |(\phi_a - \phi_{\Omega,a})(y)| \leq Ce^{-\gamma \mathrm{dist}(y, \partial\Omega)}. \tag{4.10}$$

Remark 3. *Let $R > 0$ and $R_n \uparrow \infty$, then applying Proposition 4.2, with $\Omega = B_{R_n}(0)$ and $m_\Omega = m_{R_n}$ and $0 < a \leq a_0 = a_0(\omega)$ gives a rate of convergence for the finite approximation $(u_{a,R_n}, \phi_{a,R_n})$, solving (2.3), to the ground state (u_a, ϕ_a)*

$$\|u_a - u_{a,R_n}\|_{W^{2,\infty}(B_R(0))} + \|\phi_a - \phi_{a,R_n}\|_{L^\infty(B_R(0))} \leq Ce^{-\gamma(R_n - R)}. \tag{4.11}$$

This strengthens the result that $(u_{a,R_n}, \phi_{a,R_n})$ converges to (u_a, ϕ_a) pointwise almost everywhere along a subsequence [6]. □

4.3. **Pointwise stability and neutrality estimates.** The following results extend [11, Corollary 4.2, Theorem 4.3] to the Yukawa model. Corollary 4.3 shows that the decay properties of the nuclear perturbation are inherited by the response of the Yukawa ground state, and Corollary 4.4 shows the neutrality of nuclear perturbations for the TFW equations in the Yukawa setting.

Corollary 4.3. *Let $a_0 > 0$, $k \in \mathbb{N}_0$, $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$ and $0 < a \leq a_0$, then let $(u_{1,a}, \phi_{1,a}), (u_{2,a}, \phi_{2,a})$ denote the corresponding Yukawa ground states and define*

$$w = u_{1,a} - u_{2,a}, \quad \psi = \phi_{1,a} - \phi_{2,a}, \quad R_m = 4\pi(m_1 - m_2).$$

(1) *(Exponential Decay) If $R_m \in H^k(\mathbb{R}^3)$ and $\mathrm{spt}(R_m) \subset B_R(0)$, or there exists $\gamma' > 0$ such that $\sum_{|\beta| \leq k} |\partial^\beta R_m(x)| \leq Ce^{-\gamma'|x|}$, then there exist $C = C(a_0, k, M, \omega), \gamma = \gamma(a_0, M, \omega) > 0$ depending also on R or γ' such that*

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(x)| + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(x)| \leq Ce^{-\gamma|x|}. \tag{4.12}$$

(2) *(Algebraic Decay) If there exist $C, r > 0$ such that $\sum_{|\beta| \leq k} |\partial^\beta R_m(x)| \leq C(1 + |x|)^{-r}$ then there exists $C = C(a_0, r, k, M, \omega) > 0$ such that*

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(x)| + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(x)| \leq C(1 + |x|)^{-r}. \tag{4.13}$$

(3) *(Global Estimates) If $R_m \in H^k(\mathbb{R}^3)$ then there exists $C = C(a_0, k, M, \omega) > 0$ such that*

$$\|w\|_{H^{k+4}(\mathbb{R}^3)} + \|\psi\|_{H^{k+2}(\mathbb{R}^3)} \leq C\|R_m\|_{H^k(\mathbb{R}^3)}. \tag{4.14}$$

Corollary 4.4. *Let $a_0 > 0$, $m_1, m_2 \in \mathcal{M}_{L^2}(M, \omega)$ and $0 < a \leq a_0$, then define $\rho_{12,a} := m_1 - u_{1,a}^2 - m_2 + u_{2,a}^2$.*

(1) *If* $\mathrm{spt}(m_1 - m_2) \subset B_{R'}(0)$, *or there exist* $C, \widetilde{\gamma} > 0$ *such that* $|(m_1 - m_2)(x)| \leq Ce^{-\widetilde{\gamma}|x|}$, *then* $\rho_{12,a} \in L^1(\mathbb{R}^3)$ *and there exist* $C, \gamma > 0$, *independent of* a, *such that, for all* $R > 0$,

$$\left| \int_{B_R(0)} \rho_{12,a} \right| \leq Ce^{-\gamma R}. \tag{4.15}$$

(2) *If there exists* $C, r > 0$ *such that* $|(m_1 - m_2)(x)| \leq C(1 + |x|)^{-r}$ *then there exists* $C > 0$, *independent of* a, *such that, for all* $R > 0$,

$$\left| \int_{B_R(0)} \rho_{12,a} \right| \leq C(1 + R)^{2-r}. \tag{4.16}$$

(3) *If* $m_1 - m_2 \in L^2(\mathbb{R}^3)$ *(e.g.,* $r > 3/2$ *in (2)) then* $\rho_{12,a} \in L^2(\mathbb{R}^3)$ *and*

$$\lim_{\varepsilon \to 0} \frac{1}{|B_\varepsilon(0)|} \int_{B_\varepsilon(0)} \widehat{\rho}_{12,a}(k) \; \mathrm{d}k = 0, \tag{4.17}$$

where $\widehat{\rho}_{12,a}$ *denotes the Fourier transform of* $\rho_{12,a}$.

5. Proofs

The following technical lemma is used in Proposition 5.3 to show $u_{a,R_n} > 0$ but will also be useful to show a uniform lower bound for the ground state electron density u_a in Lemma 6.1 in the Appendix.

Lemma 5.1. *Let* $0 < a_1 \leq a_2$ *and* $m \in \mathcal{M}_{L^2}(M, \omega)$, *then for* $R_n > 0$ *define* $\psi_{R_n} \in C_c^\infty(B_{4R_n}(0))$ *satisfying* $\psi_{R_n} \geq 0$ *and* $\psi_{R_n} = 1$ *on* $B_{2R_n}(0)$ *and* $m_{R_n} = m \cdot \chi_{B_{R_n}(0)}$. *Then there exists* $C_0 = C_0(a_1, a_2, \omega) > 0$ *and* $R_0 = R_0(a_1, a_2, \omega) > 0$ *such that for all* $a_1 \leq a \leq a_2$ *and* $R_n \geq R_0$

$$\int_{\mathbb{R}^3} |\nabla \psi_{R_n}|^2 - D_a(m_{R_n}, \psi_{R_n}^2) \leq -C_0 R_n^3. \tag{5.1}$$

Proof of Lemma 5.1. Let $a_1 \leq a \leq a_2$. By the construction of ψ_{R_n}

$$\int |\nabla \psi_{R_n}|^2 = \int_{B_{4R_n}(0) \smallsetminus B_{2R_n}(0)} |\nabla \psi_{R_n}|^2 \leq C \int_{B_{4R_n}(0) \smallsetminus B_{2R_n}(0)} R_n^{-2} \leq C_1 R_n. \tag{5.2}$$

Additionally, it follows that

$$\begin{aligned}
D_a(m_{R_n}, \psi_{R_n}^2) &= \int_{\mathbb{R}^3} (m_{R_n} * Y_a) \psi_{R_n}^2 \geq \int_{B_{2R_n}(0)} (m_{R_n} * Y_a)(x) \; \mathrm{d}x \\
&= \int_{\mathbb{R}^3} \left(\int_{B_{2R_n}(0) \cap B_{R_n}(y)} m_{R_n}(x - y) \; \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|} \; \mathrm{d}y \\
&= \int_{\mathbb{R}^3} \left(\int_{B_{2R_n}(-y) \cap B_{R_n}(0)} m_{R_n}(x) \; \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|} \; \mathrm{d}y.
\end{aligned} \tag{5.3}$$

First consider for $R' > 0$

$$\int_{B_{R'}(0)} \frac{e^{-a|y|}}{|y|} \; \mathrm{d}y = 4\pi \int_0^{R'} re^{-ar} \; \mathrm{d}r = \frac{4\pi}{a^2} \left(1 - e^{-aR'}(1 + aR') \right),$$

hence choosing $R' = (4a)^{-1}$ ensures that

$$\int_{B_{1/4a}(0)} \frac{e^{-a|y|}}{|y|} \; \mathrm{d}y = \frac{4\pi}{a^2} \left(1 - \tfrac{5}{4}e^{-1/4} \right) =: C_2 a^{-2}, \tag{5.4}$$

where $C_2 > 0$. Now choose $R_n \geq (4a)^{-1}$, then the triangle inequality implies for $|y| \leq (4a)^{-1}$, $B_{2R_n}(-y) \supset B_{R_n}(0)$, hence as $m \in \mathcal{M}_{L^2}(M, \omega)$

$$\int_{B_{2R_n}(-y) \cap B_{R_n}(0)} m_{R_n}(x) \, \mathrm{d}x \geq \int_{B_{R_n}(0)} m(x) \, \mathrm{d}x \geq \omega_0 R_n^3 - \omega_1. \tag{5.5}$$

Combining the inequalities (5.3)–(5.5) gives

$$\begin{aligned}
D_a(m_{R_n}, \psi_{R_n}^2) &= \int_{\mathbb{R}^3} \left(\int_{B_{2R_n}(-y) \cap B_{R_n}(0)} m_{R_n}(x) \, \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|} \, \mathrm{d}y \\
&\geq \int_{B_{1/4a}(0)} \left(\int_{B_{2R_n}(-y) \cap B_{R_n}(0)} m_{R_n}(x) \, \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|} \, \mathrm{d}y \\
&\geq \int_{B_{1/4a}(0)} \left(\int_{B_{R_n}(0)} m_{R_n}(x) \, \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|} \, \mathrm{d}y \geq C_2 a^{-2} (\omega_0 R_n^3 - \omega_1). \tag{5.6}
\end{aligned}$$

Now define $C_0 = \frac{C_2 \omega_0}{2a_2^2} > 0$ and $R_n \geq R_0 := \max\{1, (4a_1)^{-1}, (\frac{C_1 + C_2 \omega_1 a_1^{-2}}{C_0})^{1/2}\}$, then combining (5.2) and (5.6) yields the desired estimate (5.1) for any $a_1 \leq a \leq a_2$ and $R_n \geq R_0$

$$\begin{aligned}
\int |\nabla \psi_{R_n}|^2 - D_a(m_{R_n}, \psi_{R_n}^2) &\leq \left(C_1 R_n + C_2 \omega_1 a^{-2} \right) - 2C_0 R_n^3 \\
&\leq C_0 R_n^3 - 2C_0 R_n^3 = -C_0 R_n^3. \qquad \square
\end{aligned}$$

5.1. Proof of regularity estimates.

Proposition 5.2. *Let* $m : \mathbb{R} \to \mathbb{R}_{\geq 0}$ *satisfy*

$$\|m\|_{L_{\mathrm{unif}}^2(\mathbb{R}^3)} \leq M,$$

and $R_n \uparrow \infty$, *then define the truncated nuclear distribution* $m_{R_n} = m \cdot \chi_{B_{R_n}(0)}$. *There exists* $R_0 = R_0(m), a_0 = a_0(m) > 0$ *such that for all* $R_n \geq R_0$ *and* $0 < a \leq a_0$, *the unique solution to the minimisation problem*

$$I_a^{\mathrm{TFW}}(m_{R_n}) = \inf \left\{ E_a^{\mathrm{TFW}}(v, m_{R_n}) \,\middle|\, \nabla v \in L^2(\mathbb{R}^3), v \in L^{10/3}(\mathbb{R}^3), v \geq 0 \right\} \tag{5.7}$$

yields a unique solution $(u_{a,R_n}, \phi_{a,R_n})$ *to*

$$-\Delta u_{a,R_n} + \frac{5}{3} u_{a,R_n}^{7/3} - \phi_{a,R_n} u_{a,R_n} = 0, \tag{5.8a}$$

$$-\Delta \phi_{a,R_n} + a^2 \phi_{a,R_n} = 4\pi \left(m_{R_n} - u_{a,R_n}^2 \right). \tag{5.8b}$$

which satisfy the following estimates, with constants independent of R_n:

$$\|u_{a,R_n}\|_{H_{\mathrm{unif}}^4(\mathbb{R}^3)} \leq C(M), \tag{5.9}$$

$$\|\phi_{a,R_n}\|_{H_{\mathrm{unif}}^2(\mathbb{R}^3)} \leq C(M), \tag{5.10}$$

and $u_{a,R_n} > 0$ *on* $\mathbb{R}^3$ *whenever* $m_{R_n} \not\equiv 0$. *In particular, if* $\int_{B_{R_0}(x)} m \geq c_0 > 0$ *for some* $x \in \mathbb{R}^3$ *and* $R_0, c_0 > 0$, *then* $a_0 = a_0(R_0, c_0) > 0$.

In the case $m \in \mathcal{M}_{L^2}(M, \omega)$, Proposition 5.2 can be extended to all $a > 0$. The following result will be used to prove Proposition 3.1.

Proposition 5.3. *Let $a_0 > 0$, $m \in \mathcal{M}_{L^2}(M, \omega)$ and $R_n \uparrow \infty$, then define $m_{R_n} := m \cdot \chi_{B_{R_n}(0)}$. There exists $R_0 = R_0(a_0, \omega) > 0$ such that for all $0 < a \leq a_0$ and $R_n \geq R_0$, the minimisation problem (5.7) yields a unique solution $(u_{a,R_n}, \phi_{a,R_n})$ to (5.8) which satisfy the following estimates, with constants independent of a and R_n:*

$$\|u_{a,R_n}\|_{H^4_{\text{unif}}(\mathbb{R}^3)} \leq C(a_0, M), \tag{5.11}$$

$$\|\phi_{a,R_n}\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \leq C(a_0, M). \tag{5.12}$$

Remark 4. The Coulomb minimisation problem [11, Proposition 6.3] imposes a charge neutrality condition. Imposing a neutrality condition for the finite Yukawa problem introduces a Lagrange multiplier into (5.8) that weakens Theorem 3.5 significantly. □

The proof of Proposition 5.2 largely follows the proof of [11, Proposition 6.3]. Proposition 5.2 is proved in four steps.

In Step 1, the minimisation problem (5.7) is shown to be well-posed and defines a unique solution $(u_{a,R_n}, \phi_{a,R_n})$ to (5.8), where u_{a,R_n}, ϕ_{a,R_n} are continuous and decay at infinity. The argument in Step 2 adapts the Solovej estimate for Yukawa systems to show: there exists $C_S > 0$ that for all $m \in \mathcal{M}_{L^2}(M, \omega)$ and $a, R_n > 0$

$$\tfrac{10}{9} u_{a,R_n}^{4/3} \leq \phi_{a,R_n} + C_S + a^2. \tag{5.13}$$

The aim of Step 3 is to show that there exists $a_0 = a_0(\omega), R_0 = R_0(\omega) > 0$ such that for all $0 < a \leq a_0 \leq 1$ and $R_n \geq R_0$

$$u_{a,R_n} > 0 \quad \text{on } \mathbb{R}^3.$$

Finally, in Step 4, the following estimate is established

$$\|u_{R_n}\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \|\phi_{R_n}\|_{L^\infty(\mathbb{R}^3)} \leq C(M) + a^2 \leq C(M) + 1, \tag{5.14}$$

where the final constant is independent of a, a_0 and R_n. The desired estimates (5.9)-(5.10) then follow from standard elliptic regularity.

Proof of Proposition 5.2. If $m \equiv 0$, then for all $a > 0$ and R_n, clearly $u_{a,R_n} = \phi_{a,R_n} = m_{R_n} = 0$ satisfies (5.8) and (5.9)–(5.10).

If $m \not\equiv 0$, then $\int_{B_{R_0}(x)} m \geq c_0 > 0$ for some $x \in \mathbb{R}^3$ and $R_0, c_0 > 0$. Without loss of generality suppose $x = 0$ otherwise translate m.

Step 1 For each $n \in \mathbb{N}$ define

$$m_{R_n}(x) = m(x) \cdot \chi_{B_{R_n}}(x),$$

and choosing $R_n \geq R_0$ ensures that $\int_{\mathbb{R}^3} m_{R_n} \geq c_0 > 0$, hence $m_{R_n} \not\equiv 0$. Recall

$$E_a^{\text{TFW}}(v, m_{R_n}) = \int |\nabla v|^2 + \int v^{10/3} + \frac{1}{2} D_a(m_{R_n} - v^2, m_{R_n} - v^2) \geq 0.$$

For each R_n and $a > 0$, recall the minimisation problem (5.7)

$$I_a^{\text{TFW}}(m_{R_n}) = \inf \left\{ E_a^{\text{TFW}}(v, m_{R_n}) \,\middle|\, \nabla v \in L^2(\mathbb{R}^3), v \in L^{10/3}(\mathbb{R}^3), v \geq 0 \right\}.$$

By the Gagliardo–Nirenberg–Sobolev embedding [9], $v \in L^6(\mathbb{R}^3)$ and $\|v\|_{L^6(\mathbb{R}^3)} \leq C\|\nabla v\|_{L^2(\mathbb{R}^3)}$, moreover $v \in L^p(\mathbb{R}^3)$ for $p \in [10/3, 6]$. Consequently

$$0 \leq D_a(v^2, v^2) \leq \|Y_a\|_{L^1(\mathbb{R}^3)} \|v\|_{L^4(\mathbb{R}^3)}^4 \leq C\|v\|_{L^{10/3}(\mathbb{R}^3)}^{5/2} \|v\|_{L^6(\mathbb{R}^3)}^{3/2} \leq C\|v\|_{L^{10/3}(\mathbb{R}^3)}^{5/2} \|\nabla v\|_{L^2(\mathbb{R}^3)}^{3/2}.$$

Observe that there are no charge constraints on the electron density as in general $v \notin L^2(\mathbb{R}^3)$. This is chosen to ensure that no Lagrange multipliers appear in (5.8).

As $m_{R_n} \in L^{p_1}(\mathbb{R}^3), Y_a \in L^{p_2}(\mathbb{R}^3)$ for all $p_1 \in [1, 2], p_2 \in [1, 3)$, applying Young's inequality yields

$$D_a(m_{R_n}, v^2) \leq \|Y_a\|_{L^{5/2}(\mathbb{R}^3)} \|m_{R_n}\|_{L^1(\mathbb{R}^3)} \|v^2\|_{L^{5/3}(\mathbb{R}^3)} \leq C\|v\|^2_{L^{10/3}(\mathbb{R}^3)} \leq C + \frac{1}{2}\|v\|^{10/3}_{L^{10/3}(\mathbb{R}^3)},$$

it follows that

$$E_a^{\text{TFW}}(v, m_{R_n}) \geq \frac{1}{2}\left(\|\nabla v\|^2_{L^2(\mathbb{R}^3)} + \|v\|^{10/3}_{L^{10/3}(\mathbb{R}^3)} + D_a(v^2, v^2)\right) + \frac{1}{2}D_a(m_{R_n}, m_{R_n}) - C.$$

As the energy is bounded below, there exists a minimising sequence v_k satisfying

$$\|\nabla v\|^2_{L^2(\mathbb{R}^3)} + \|v\|^{10/3}_{L^{10/3}(\mathbb{R}^3)} + D_a(v^2, v^2) \leq C,$$

hence there exists u_{a,R_n} such that $\nabla u_{a,R_n} \in L^2(\mathbb{R}^3), u_{a,R_n} \in L^{10/3}(\mathbb{R}^3)$. Moreover, along a subsequence ∇v_k converges to $\nabla u_{a,R_n}$ weakly in $L^2(\mathbb{R}^3)$, v_k converges to u_{a,R_n}, weakly in $L^6(\mathbb{R}^3)$ and $L^{10/3}(\mathbb{R}^3)$, strongly in $L^p(B_R(0))$ for all $p \in [1, 6)$ and $R > 0$ and pointwise almost everywhere. Consequently,

$$E_a^{\text{TFW}}(u_{a,R_n}, m_{R_n}) \leq \liminf_{k \to \infty} E_a^{\text{TFW}}(v_k, m_{R_n}) = I_a^{\text{TFW}}(m_{R_n}),$$

hence u_{a,R_n} is a minimiser of (5.7). Define the alternate minimisation problem

$$\inf\left\{E_a^{\text{TFW}}(\sqrt{\rho}, m_{R_n}) \,\middle|\, \nabla\sqrt{\rho} \in L^2(\mathbb{R}^3), \rho \in L^{5/3}(\mathbb{R}^3), \rho \geq 0\right\}. \tag{5.15}$$

Due to the strict convexity of $\rho \mapsto E_a^{\text{TFW}}(\sqrt{\rho}, m_{R_n})$, it follows that $\rho_{a,R_n} = u_{a,R_n}^2$ is the unique minimiser of (5.15), hence u_{a,R_n} is the unique minimiser of (5.7).

Define

$$\phi_{a,R_n} = (m_{R_n} - u_{a,R_n}^2) * Y_a, \tag{5.16}$$

then it follows that $(u_{a,R_n}, \phi_{a,R_n})$ is the unique distributional solution to (5.8)

$$-\Delta u_{a,R_n} + \frac{5}{3}u_{a,R_n}^{7/3} - \phi_{a,R_n} u_{a,R_n} = 0,$$

$$-\Delta\phi_{a,R_n} + a^2\phi_{a,R_n} = 4\pi\left(m_{R_n} - u_{a,R_n}^2\right).$$

Moreover, as $m_{R_n} - u_{a,R_n}^2 \in L^2(\mathbb{R}^3)$ and the Fourier transform of Y_a, $\widehat{Y_a}$, satisfies

$$\widehat{Y_a}(k) = \frac{1}{a^2 + |k|^2},$$

it follows that

$$\int_{\mathbb{R}^3} |\widehat{\phi_{a,R_n}}(k)|^2(a^2 + |k|^2)\,\mathrm{d}k = \int_{\mathbb{R}^3} |\widehat{(m_{R_n} - u_{a,R_n}^2)}(k)|^2|\widehat{Y_a}(k)|^2(a^2 + |k|^2)\,\mathrm{d}k$$

$$= \int_{\mathbb{R}^3} \frac{|\widehat{(m_{R_n} - u_{a,R_n}^2)}(k)|^2}{(a^2 + |k|^2)}\,\mathrm{d}k$$

$$= \int_{\mathbb{R}^3}\left((m_{R_n} - u_{a,R_n}^2) * Y_a\right)(m_{R_n} - u_{a,R_n}^2)$$

$$= D_a(m_{R_n} - u_{a,R_n}^2, m_{R_n} - u_{a,R_n}^2).$$

It follows that $\phi_{a,R_n} \in H^1(\mathbb{R}^3)$ and

$$\int_{\mathbb{R}^3} |\nabla\phi_{a,R_n}|^2 + a^2\int_{\mathbb{R}^3}\phi_{a,R_n}^2 = D_a(m_{R_n} - u_{a,R_n}^2, m_{R_n} - u_{a,R_n}^2). \tag{5.17}$$

Additionally, by applying Young's inequality yields

$$\|\phi_{a,R_n}\|_{L^\infty(\mathbb{R}^3)} \leq \|m_{R_n}\|_{L^2(\mathbb{R}^3)}\|Y_a\|_{L^2(\mathbb{R}^3)} + \leq \|u_{a,R_n}^2\|_{L^3(\mathbb{R}^3)}\|Y_a\|_{L^{3/2}(\mathbb{R}^3)}$$
$$\leq \|m_{R_n}\|_{L^2(\mathbb{R}^3)}\|Y_a\|_{L^2(\mathbb{R}^3)} + \leq \|u_{a,R_n}\|_{L^6(\mathbb{R}^3)}^2\|Y_a\|_{L^{3/2}(\mathbb{R}^3)},$$

hence by [16, Lemma II.25], ϕ_{a,R_n} is a bounded, continuous function that decays uniformly at infinity. In addition, as $m_{R_n} \in L^p(\mathbb{R}^3)$ for all $p \in [1,2]$, $Y_a \in L^1(\mathbb{R}^3)$ and $u_{a,R_n} \in L^{10/3}(\mathbb{R}^3)$, it follows that

$$\|\phi_{a,R_n}\|_{L^{5/3}(\mathbb{R}^3)} \leq \|m_{R_n} - u_{a,R_n}^2\|_{L^{5/3}(\mathbb{R}^3)}\|Y_a\|_{L^1(\mathbb{R}^3)}$$
$$\leq C\left(\|m_{R_n}\|_{L^{5/3}(\mathbb{R}^3)} + \|u_{a,R_n}^2\|_{L^{5/3}(\mathbb{R}^3)}\right)$$
$$\leq C\left(\|m_{R_n}\|_{L^{5/3}(\mathbb{R}^3)} + \|u_{a,R_n}\|_{L^{10/3}(\mathbb{R}^3)}^2\right).$$

To bound u_{a,R_n} above, recall that u_{a,R_n} solves

$$-\Delta u_{a,R_n} = -\frac{5}{3}u_{a,R_n}^{7/3} + \phi_{a,R_n}u_{a,R_n}, \tag{5.18}$$

and $u_{a,R_n} \in L^{10/3}(\mathbb{R}^3) \cap L^6(\mathbb{R}^3), \phi_{a,R_n} \in L^{5/3}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. It follows that the right-hand side of (5.18) belongs to $L^2(\mathbb{R}^3)$ and

$$\| -\tfrac{5}{3}u_{a,R_n}^{7/3} + \phi_{a,R_n}u_{a,R_n}\|_{L^2(\mathbb{R}^3)} \leq \tfrac{5}{3}\|u_{a,R_n}^{7/3}\|_{L^2(\mathbb{R}^3)} + \|\phi_{a,R_n}u_{a,R_n}\|_{L^2(\mathbb{R}^3)}$$
$$\leq \tfrac{5}{3}\|u_{a,R_n}\|_{L^{14/3}(\mathbb{R}^3)}^{7/3} + \|\phi_{a,R_n}\|_{L^5(\mathbb{R}^3)}\|u_{a,R_n}\|_{L^{10/3}(\mathbb{R}^3)}$$
$$\leq \tfrac{5}{3}\|u_{a,R_n}\|_{L^{10/3}(\mathbb{R}^3)}^{5/6}\|u_{a,R_n}\|_{L^6(\mathbb{R}^3)}^{3/2} + \|\phi_{a,R_n}\|_{L^5(\mathbb{R}^3)}\|u_{a,R_n}\|_{L^{10/3}(\mathbb{R}^3)}.$$

Then for any $x \in \mathbb{R}^3$ applying the elliptic regularity estimate [9] yields

$$\|u_{a,R_n}\|_{H^2(B_1(x))} \leq C(\|\tfrac{5}{3}u_{a,R_n}^{7/3} - \phi_{a,R_n}u_{a,R_n}\|_{L^2(B_2(x))} + \|u_{a,R_n}\|_{L^2(B_2(x))})$$
$$\leq C(\|\tfrac{5}{3}u_{a,R_n}^{7/3} - \phi_{a,R_n}u_{a,R_n}\|_{L^2(\mathbb{R}^3)} + \|u_{a,R_n}\|_{L^{10/3}(B_2(x))})$$
$$\leq C(\|\tfrac{5}{3}u_{a,R_n}^{7/3} - \phi_{a,R_n}u_{a,R_n}\|_{L^2(\mathbb{R}^3)} + \|u_{a,R_n}\|_{L^{10/3}(\mathbb{R}^3)}),$$

where the constant is independent of $x \in \mathbb{R}^3$. The Sobolev embedding $H^2(B_1(x)) \hookrightarrow C^{0,1/2}(B_1(x))$ implies that u_{a,R_n} is continuous and bounded as

$$\|u_{a,R_n}\|_{L^\infty(B_1(x))} \leq \|u_{a,R_n}\|_{C^{0,1/2}(B_1(x))} \leq C\|u_{a,R_n}\|_{H^2(B_1(x))},$$

hence

$$\|u_{a,R_n}\|_{L^\infty(\mathbb{R}^3)} = \sup_{x \in \mathbb{R}^3}\|u_{a,R_n}\|_{L^\infty(B_1(x))} \leq \sup_{x \in \mathbb{R}^3} C\|u_{a,R_n}\|_{H^2(B_1(x))} < \infty. \tag{5.19}$$

It remains to show that u_{a,R_n} decays at infinity. Recall that u_{a,R_n} solves (5.18)

$$-\Delta u_{R_n} = -\frac{5}{3}u_{R_n}^{7/3} + \phi_{R_n}u_{R_n}$$

and also that $u_{a,R_n} \in L^{10/3}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3), \phi_{a,R_n} \in L^{5/3}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. Define

$$g_{a,R_n} := \left(-\frac{5}{3}u_{a,R_n}^{7/3} + \phi_{a,R_n}u_{a,R_n}\right) * \frac{1}{|\cdot|}. \tag{5.20}$$

Observe that $u_{a,R_n}^{7/3} \in L^{10/7}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ and applying Hölder's inequality gives

$$\|\phi_{a,R_n}u_{a,R_n}\|_{L^{10/9}(\mathbb{R}^3)} \leq \|\phi_{a,R_n}\|_{L^{5/3}(\mathbb{R}^3)}\|u_{a,R_n}\|_{L^{10/3}(\mathbb{R}^3)},$$

hence $\phi_{a,R_n} u_{a,R_n} \in L^{10/9}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. It follows that $-\frac{5}{3} u_{R_n}^{7/3} + \phi_{R_n} u_{R_n} \in L^{10/7}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. Decompose

$$g_{a,R_n} = \left(-\frac{5}{3} u_{a,R_n}^{7/3} + \phi_{a,R_n} u_{a,R_n} \right) * \left(\frac{1}{|\cdot|} \chi_{B_1(0)} \right) + \left(-\frac{5}{3} u_{a,R_n}^{7/3} + \phi_{a,R_n} u_{a,R_n} \right) * \left(\frac{1}{|\cdot|} \chi_{B_1(0)^c} \right),$$

then as $\frac{1}{|\cdot|} \chi_{B_1(0)} \in L^{p_1}(\mathbb{R}^3)$ for all $p_1 \in [1,3)$, $\frac{1}{|\cdot|} \chi_{B_1^c(0)} \in L^{p_2}(\mathbb{R}^3)$ for all $p_2 \in (3,\infty]$ applying Young's inequality yields

$$\|g_{a,R_n}\|_{L^\infty(\mathbb{R}^3)} \leq \|\tfrac{5}{3} u_{a,R_n}^{7/3} - \phi_{a,R_n} u_{a,R_n}\|_{L^2(\mathbb{R}^3)} \left\| \tfrac{1}{|\cdot|} \chi_{B_1(0)} \right\|_{L^2(\mathbb{R}^3)}$$
$$+ \|\tfrac{5}{3} u_{a,R_n}^{7/3} - \phi_{a,R_n} u_{a,R_n}\|_{L^{10/7}(\mathbb{R}^3)} \left\| \tfrac{1}{|\cdot|} \chi_{B_1(0)^c} \right\|_{L^{10/3}(\mathbb{R}^3)},$$

hence [16, Lemma II.25] implies that g_{a,R_n} is a continuous, bounded function vanishing at infinity. In addition, g_{a,R_n} solves

$$-\Delta g_{a,R_n} = -\frac{5}{3} u_{a,R_n}^{7/3} + \phi_{a,R_n} u_{a,R_n} \tag{5.21}$$

in distribution. Combining (5.18) and (5.21), it follows that

$$-\Delta(u_{a,R_n} - g_{a,R_n}) = 0,$$

in distribution, so by Weyl's Lemma $u_{a,R_n} - g_{a,R_n}$ is harmonic [12]. As $u_{a,R_n} - g_{a,R_n} \in L^\infty(\mathbb{R}^3)$, Liouville's Theorem implies $u_{a,R_n} - g_{a,R_n}$ is constant [12]. Suppose that $u_{a,R_n} - g_{a,R_n} = c \neq 0$, then as g_{a,R_n} decays at infinity

$$\lim_{x \to \infty} u_{a,R_n}(x) = c \neq 0,$$

which contradicts $u_{a,R_n} \in L^{10/3}(\mathbb{R}^3)$. It follows that $u_{a,R_n} = g_{a,R_n}$ hence u_{a,R_n} decays uniformly at infinity.

Step 2 The argument in [18] is now adapted to show the Solovej estimate for Yukawa systems (5.13)

$$\tfrac{10}{9} u_{a,R_n}^{4/3} \leq \phi_{a,R_n} + C_S + a^2.$$

For convenience, in the following argument $u_{a,R_n}, \phi_{a,R_n}, m_{a,R_n}$ will be denoted as u, ϕ, m. As u solves (5.8a)

$$-\Delta u + \frac{5}{3} u^{7/3} - \phi u = 0,$$

following the proof of [18, Proposition 8], $w = u^{4/3}$ is non-negative and satisfies

$$-\Delta w + \frac{4}{3} \left(\tfrac{5}{3} w - \phi \right) w \leq 0. \tag{5.22}$$

Let $\lambda \in (0, \frac{5}{3})$ and define

$$v(x) = \lambda u^{4/3} - \phi - (C(\lambda) + a^2),$$

where $C(\lambda) = (9/4)\pi^2 \lambda^{-2} (\tfrac{5}{3} - \lambda)^{-1} > 0$. The expression (5.8b) can be written as

$$-\Delta \phi + a^2 \phi = 4\pi(m - w^{3/2}). \tag{5.23}$$

Combining (5.22) and (5.23), it follows that

$$\Delta v(x) \geq \frac{4\lambda}{3} \left(\tfrac{5}{3} w - \phi \right) w - 4\pi w^{3/2} + 4\pi m - a^2 \phi.$$

The aim is to prove that $v \leq 0$ by showing that $S = \{x \,|\, v(x) > 0\}$ is empty. As u, ϕ are continuous functions decaying at infinity, it follows that v is continuous, S is bounded, open and $v = 0$ on ∂S. Over S,

$$\Delta v \geq \frac{4\lambda}{3}\left(v + \tfrac{5}{3}w - \lambda w + (C(\lambda) + a^2)\right)w - 4\pi w^{3/2} + 4\pi m - a^2\phi$$

$$\geq \frac{4\lambda}{3}\left(\tfrac{5}{3}w - \lambda w + C(\lambda) + a^2\right)w - 4\pi w^{3/2} + 4\pi m - a^2\phi$$

$$= \left(\frac{4\lambda(\tfrac{5}{3} - \lambda)}{3}w - 4\pi w^{1/2} + \frac{4\lambda}{3}C(\lambda)\right)w + \frac{4\lambda}{3}a^2 w + 4\pi m - a^2\phi.$$

The value of $C(\lambda)$ is chosen to ensure that

$$\frac{4\lambda(\tfrac{5}{3} - \lambda)}{3}w - 4\pi w^{1/2} + \frac{4\lambda}{3}C(\lambda) \geq 0,$$

hence as m is non-negative and $v \geq 0$ in S

$$\Delta v \geq \frac{4\lambda}{3}a^2 w + 4\pi m - a^2\phi$$

$$\geq a^2(\lambda w - \phi) = a^2(v + (C(\lambda) + a^2)) \geq a^2(C(\lambda) + a^2) \geq 0.$$

As v satisfies

$$-\Delta v \leq 0 \quad \text{in } S,$$
$$v = 0 \quad \text{on } \partial S,$$

it follows that both $v \leq 0$ and $v > 0$ on S, hence S is non-empty and $v \leq 0$ on $\mathbb{R}^3$. So for all $\lambda \in (0, \tfrac{5}{3})$ and all $x \in \mathbb{R}^3$

$$\lambda u^{4/3}(x) \leq \phi(x) + C(\lambda) + a^2.$$

The right-hand side is minimised by choosing $\lambda = \frac{10}{9}$, which yields the desired estimate (5.13).

Step 3 The aim is to show that there exists $a_0 = a_0(\omega), R_0 = R_0(\omega) > 0$ such that for all $0 < a \leq a_0$ and $R_n \geq R_0$, $u_{a,R_n} > 0$ on $\mathbb{R}^3$, by following the argument used in [6, Proposition 2.2].

First recall the energy minimisation problem (5.7)

$$I_a^{\mathrm{TFW}}(m_{R_n}) = \inf\left\{ E_a^{\mathrm{TFW}}(v, m_{R_n}) \,\middle|\, \nabla v \in L^2(\mathbb{R}^3), v \in L^{10/3}(\mathbb{R}^3), v \geq 0 \right\}$$

where

$$E_a^{\mathrm{TFW}}(v, m_{R_n}) = \int_{\mathbb{R}^3} |\nabla v|^2 + \int_{\mathbb{R}^3} v^{10/3} + \frac{1}{2}D_a(m_{R_n} - v^2, m_{R_n} - v^2). \tag{5.24}$$

By showing that for large R_n and small $a > 0$

$$I_a^{\mathrm{TFW}}(m_{R_n}) = E_a^{\mathrm{TFW}}(u_{a,R_n}, m_{R_n}) < E_a^{\mathrm{TFW}}(0, m_{R_n}), \tag{5.25}$$

it follows that $u_{a,R_n} \not\equiv 0$, hence by the Harnack inequality $u_{a,R_n} > 0$ on $\mathbb{R}^3$ [12]. An admissible test function φ_a is constructed to satisfy: for sufficiently large R_n

$$I_a^{\mathrm{TFW}}(m_{R_n}) \leq E_a^{\mathrm{TFW}}(\varphi_{a_0}, m_{R_n}) < E_a^{\mathrm{TFW}}(0, m_{R_n}) = \frac{1}{2}D_a(m_{R_n}, m_{R_n}).$$

For $\varepsilon > 0$, let $\varphi_a = \varepsilon \psi_a$ and consider the difference

$$E_a^{\mathrm{TFW}}(\varepsilon \psi_a, m_{R_n}) - E_a^{\mathrm{TFW}}(0, m_{R_n})$$
$$= \varepsilon^2 \left(\int |\nabla \psi_a|^2 - D_a(m_{R_n}, \psi_a^2) \right) + \frac{\varepsilon^4}{2} D_a(\psi_a^2, \psi_a^2) + \varepsilon^{10/3} \int \psi_a^{10/3}. \tag{5.26}$$

For small $\varepsilon > 0$, the right-hand side of (5.26) is shown to be negative by first proving that there exists $a_0, C_0 > 0$ such that for all $0 < a \leq a_0$

$$\int_{\mathbb{R}^3} |\nabla \psi_a|^2 - D_a(m_{R_n}, \psi_a^2) \leq -\frac{C_0}{2} a < 0. \tag{5.27}$$

Let $\psi_0 \in C_c^\infty(B_1(0))$ satisfy $\psi_0 \geq 0$, and $\psi_0 = 1$ on $B_{1/2}(0)$, then define $\psi_a(x) = a^{3/2} \psi_0(ax)$, for $a \in (0, 1]$.

Using the definition of ψ_a gives

$$D_a(m_{R_n}, \psi_a^2) = \int_{\mathbb{R}^3} (m_{R_n} * Y_a) \psi_a^2 \geq \frac{a^3}{4} \int_{B_{1/2a}(0)} (m_{R_n} * Y_a)(x)\, \mathrm{d}x$$

$$= a^3 \int_{\mathbb{R}^3} \left(\int_{B_{1/2a}(0) \cap B_{R_n}(y)} m_{R_n}(x - y)\, \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|}\, \mathrm{d}y$$

$$= a^3 \int_{\mathbb{R}^3} \left(\int_{B_{1/2a}(-y) \cap B_{R_n}(0)} m_{R_n}(x)\, \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|}\, \mathrm{d}y. \tag{5.28}$$

First consider for $R' > 0$

$$\int_{B_{R'}(0)} \frac{e^{-a|y|}}{|y|}\, \mathrm{d}y = 4\pi \int_0^{R'} r e^{-ar}\, \mathrm{d}r = \frac{4\pi}{a^2} \left(1 - e^{-aR'}(1 + aR') \right),$$

hence choosing $R' = (4a)^{-1}$ ensures that

$$\int_{B_{1/4a}(0)} \frac{e^{-a|y|}}{|y|}\, \mathrm{d}y = \frac{4\pi}{a^2} \left(1 - \tfrac{5}{4} e^{-1/4} \right) \geq \frac{\pi}{10 a^2}. \tag{5.29}$$

Now choose $a^* = \min\{1, (4R_0)^{-1}\}$ and suppose $R_n \geq R_0$. Then for all $y \in B_{1/4a}(0)$, it follows from the triangle inequality that $B_{R_0}(0) \subset B_{1/2a}(-y) \cap B_{R_n}(0)$, hence

$$\int_{B_{1/2a}(-y) \cap B_{R_n}(0)} m_{R_n}(x)\, \mathrm{d}x \geq \int_{B_{R_0}(0)} m(x)\, \mathrm{d}x \geq c_0 > 0. \tag{5.30}$$

Applying (5.29)–(5.30) to (5.28), it follows that for all $0 < a \leq a^*$ and $R_n \geq R_0$

$$D_a(m_{R_n}, \psi_a^2) = \int_{\mathbb{R}^3} (m_{R_n} * Y_a) \psi_a^2$$

$$\geq a^3 \int_{\mathbb{R}^3} \left(\int_{B_{1/2a}(-y) \cap B_{R_n}(0)} m_{R_n}(x)\, \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|}\, \mathrm{d}y$$

$$= c_0 a^3 \int_{B_{1/4a}(0)} \frac{e^{-a|y|}}{|y|}\, \mathrm{d}y \geq \frac{c_0 \pi}{10} a =: C_0\, a. \tag{5.31}$$

Using a change of variables

$$\int_{B_{1/a}(0)} |\nabla \psi_a|^2 = a^2 \int_{B_1(0)} |\nabla \psi_0|^2 =: C_1 a^2. \tag{5.32}$$

Now define $a_0 = \min\{a^*, \frac{C_0}{2C_1}\}$, then for any $0 < a \le a_0$ and $R_n \ge R_0$, combining (5.31)–(5.32) yields (5.27)

$$\int |\nabla \psi_a|^2 - D_a(m_{R_n}, \psi_a^2) \le C_1 a^2 - C_0 a \le \frac{C_0}{2} a - C_0 a = -\frac{C_0}{2} a < 0.$$

Using that $a_0, \varepsilon \in (0, 1]$, the remaining terms in (5.26) can be estimated using a change of variables

$$\frac{\varepsilon^4}{2} D_a(\psi_{a_0}^2, \psi_{a_0}^2) + \varepsilon^{10/3} \int \psi_{a_0}^{10/3} = \frac{\varepsilon^4 a_0}{2} D_0(\psi_0^2, \psi_0^2) + \varepsilon^{10/3} a_0^7 \int \psi_0^{10/3}$$

$$\le \left(\frac{1}{2} D_0(\psi_0^2, \psi_0^2) + \int \psi_0^{10/3}\right) \varepsilon^4 a_0 =: C_2 \varepsilon^4 a_0. \tag{5.33}$$

Applying the estimates (5.27)-(5.33) to (5.26) and choosing $0 < \varepsilon \le \min\{1, (\frac{C_0}{3C_2})^{1/2}\}$ yields the desired result (5.25)

$$E_a^{\mathrm{TFW}}(\varepsilon \psi_a, m_{R_n}) - E_a^{\mathrm{TFW}}(0, m_{R_n}) \le \left(C_2 \varepsilon^2 - \frac{C_0}{2}\right) \varepsilon^2 a_0 < 0.$$

Step 4 The aim is to show a uniform upper bound for ϕ_{a,R_n}, which together with (5.13) yields the uniform estimate (5.14)

$$\|u_{a,R_n}\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \|\phi_{a,R_n}\|_{L^\infty(\mathbb{R}^3)} \le C(M) + a^2 \le C(M) + 1,$$

where the constant is independent of a and R_n. This will be proved by adapting the argument used to show uniform regularity for finite systems with Coulomb interaction [11, 6].

As $u_{a,R_n} \ge 0$, re-arranging the Solovej estimate (5.13) gives the uniform lower bound

$$\phi_{a,R_n} \ge -(C_S + a^2). \tag{5.34}$$

If ϕ_{a,R_n} is non-positive, then (5.14) holds as

$$\|u_{a,R_n}\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \|\phi_{a,R_n}\|_{L^\infty(\mathbb{R}^3)} \le 2(C_S + a^2) \le 2(C_S + 1).$$

Instead, suppose that ϕ_{a,R_n}^+ is non-zero at some point in $\mathbb{R}^3$. As shown in Step 1, ϕ_{a,R_n} is a continuous function that decays at infinity, hence there exists $x_{a,R_n} \in \mathbb{R}^3$ such that

$$\phi_{a,R_n}^+(x_{a,R_n}) = \|\phi_{a,R_n}^+\|_{L^\infty(\mathbb{R}^3)} > 0. \tag{5.35}$$

Without loss of generality, assume that $x_{a,R_n} = 0$.

In Step 1, it was shown that $u_{a,R_n}, \phi_{a,R_n} \in L^\infty(\mathbb{R}^3), \nabla u_{a,R_n} \in L^2(\mathbb{R}^3), \phi_{a,R_n} \in H^1(\mathbb{R}^3)$. Consequently, applying [11, Lemma 6.1] implies that $L_{a,R_n} = -\Delta + \frac{5}{3} u_{a,R_n}^{4/3} - \phi_{a,R_n}$ is a non-negative operator.

Choose $\varphi \in C_c^\infty(B_1(0))$ satisfying $0 \le \varphi \le 1$, $\varphi = 1$ on $B_{1/2}(0)$ and $\int_{\mathbb{R}^3} \varphi^2 = 1$, then for $y \in \mathbb{R}^3$, define $\varphi_y \in C_c^\infty(B_1(y))$ by $\varphi_y = \varphi(\cdot - y)$. As L_{a,R_n} is non-negative

$$\langle \varphi_y, L_{a,R_n} \varphi_y \rangle = \int_{\mathbb{R}^3} |\nabla \varphi_y|^2 + \int_{\mathbb{R}^3} \left(\frac{5}{3} u_{a,R_n}^{4/3} - \phi_{a,R_n}\right) \varphi_y^2 \ge 0,$$

which can be re-arranged and expressed using convolutions as

$$\frac{5}{3}\left(u_{a,R_n}^{4/3} * \varphi^2\right) \ge \left(\phi_{a,R_n} * \varphi^2 - \int_{\mathbb{R}^3} |\nabla \varphi|^2\right)_+$$

$$= \left(\phi_{a,R_n} * \varphi^2 - C\right)_+ \tag{5.36}$$

Observe that $\phi_{a,R_n} * \varphi^2$ solves

$$-\Delta \left(\phi_{a,R_n} * \varphi^2 \right) + a^2 \left(\phi_{a,R_n} * \varphi^2 \right) = 4\pi \left(m_{R_n} * \varphi^2 - u_{a,R_n}^2 * \varphi^2 \right). \tag{5.37}$$

The first term can be estimated uniformly

$$\left(m_{R_n} * \varphi^2 \right)(x) = \int_{B_1(x)} m_{R_n}(y) \varphi^2(x-y) \, \mathrm{d}y$$

$$\leq \int_{B_1(x)} m(y) \, \mathrm{d}y \leq C_0 \|m\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C_0 M. \tag{5.38}$$

For the second term, using the convexity of $t \mapsto t^{3/2}$ for $t \geq 0$ and the fact that $\int \varphi^2 = 1$, applying Jensen's inequality and (5.36) implies that

$$4\pi \, u_{a,R_n}^2 * \varphi^2(x) \geq \frac{5}{3} u_{a,R_n}^2 * \varphi^2(x)$$

$$= \frac{5}{3} \int_{\mathbb{R}^3} u_{a,R_n}^2(x-y) \varphi^2(y) \, \mathrm{d}y$$

$$= \frac{5}{3} \int_{\mathbb{R}^3} \left(u_{a,R_n}^{4/3}(x-y) \right)^{3/2} \varphi^2(y) \, \mathrm{d}y$$

$$\geq \frac{5}{3} \left(\int_{\mathbb{R}^3} u_{a,R_n}^{4/3}(x-y) \varphi^2(y) \, \mathrm{d}y \right)^{3/2}$$

$$= \frac{5}{3} (u_{a,R_n}^{4/3} * \varphi^2)^{3/2} \geq \left(\phi_{a,R_n} * \varphi^2 - C \right)_+^{3/2}. \tag{5.39}$$

Combining the estimates (5.37)–(5.39) yields

$$-\Delta \left(\phi_{a,R_n} * \varphi^2 \right) + a^2 \left(\phi_{a,R_n} * \varphi^2 \right) + \left(\phi_{a,R_n} * \varphi^2 - C \right)_+^{3/2} \leq C_0 M.$$

Observe that as ϕ_{a,R_n} is a continuous function that decays at infinity, $\phi_{a,R_n} * \varphi^2$ also shares these properties. Now consider the set

$$S = \{ \, x \in \mathbb{R}^3 \mid \phi_{a,R_n} * \varphi^2 - C > 0 \, \},$$

it follows that S is open and bounded and that $\phi_{a,R_n} * \varphi^2 - C = 0$ on ∂S. Observe that the constant function $h = (C_0 M)^{2/3}$ satisfies

$$-\Delta h + a^2(h + C) + h_+^{3/2} \geq h_+^{3/2} = C_0 M \quad \text{on } S,$$

$$0 = \phi_{a,R_n} * \varphi^2 - C \leq h \quad \text{in } \partial S,$$

so by the maximum principle $\phi_{a,R_n} * \varphi^2 \leq C(1 + M^{2/3})$ over S, and also on S^c, hence

$$\phi_{a,R_n} * \varphi^2 \leq C(1 + M^{2/3}). \tag{5.40}$$

Applying (5.34), it follows that

$$\phi_{a,R_n}^+ * \varphi^2 = \phi_{a,R_n}^- * \varphi^2 + \phi_{a,R_n} * \varphi^2 \leq C_S + a^2 + C(1 + M^{2/3}) = C(1 + M^{2/3}) + a^2. \tag{5.41}$$

Additionally,

$$-\Delta \phi_{a,R_n}^+ \leq -\Delta \phi_{a,R_n}^+ + a^2 \phi_{a,R_n}^+ = \left(-\Delta \phi_{a,R_n} + a^2 \phi_{a,R_n} \right) \chi_{\{\phi_{a,R_n} > 0\}}$$

$$= 4\pi \left(m_{R_n} - u_{a,R_n}^2 \right) \chi_{\{\phi_{a,R_n} > 0\}} \leq 4\pi m_{R_n} \chi_{\{\phi_{a,R_n} > 0\}} \leq 4\pi m_{R_n}. \tag{5.42}$$

From this point onwards, following the proof of [11, Proposition 6.2] verbatim with the estimates (5.41)–(5.42) gives

$$\|\phi_{a,R_n}^+\|_{L^\infty(\mathbb{R}^3)} \leq C(1 + M) + a^2. \tag{5.43}$$

Combining (5.34)–(5.43) with the Solovej estimate (5.13), yields the desired estimate (5.14)

$$\|u_{a,R_n}\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \|\phi_{a,R_n}\|_{L^\infty(\mathbb{R}^3)} \leq C(1+M) + a^2 \leq C(1+M).$$

Then, as in the proof of [11, Proposition 6.2], applying elliptic regularity estimates to the system (5.8) yields the desired estimates (5.9)–(5.10).

$$\|u_{a,R_n}\|_{H^4_{\text{unif}}(\mathbb{R}^3)} \leq C(M),$$
$$\|\phi_{a,R_n}\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \leq C(M). \qquad \square$$

Proof of Proposition 5.3. The proof follows the steps used to show Proposition 5.2. Steps 1, 2 and 4 hold verbatim and Step 3 is modified to instead show that for any $a_0 > 0$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, there exists $R_0 = R_0(a_0, \omega) > 0$ such that for any $0 < a \leq a_0$ and $R_n \geq R_0$, the unique minimiser u_{a,R_n} of (5.7) satisfies

$$u_{a,R_n} > 0 \text{ on } \mathbb{R}^3. \tag{5.44}$$

Recall the energy minimisation problem (5.7)

$$I_a^{\text{TFW}}(m_{R_n}) = \inf \left\{ E_a^{\text{TFW}}(v, m_{R_n}) \,\middle|\, \nabla v \in L^2(\mathbb{R}^3), v \in L^{10/3}(\mathbb{R}^3), v \geq 0 \right\}$$

where

$$E_a^{\text{TFW}}(v, m_{R_n}) = \int_{\mathbb{R}^3} |\nabla v|^2 + \int_{\mathbb{R}^3} v^{10/3} + \frac{1}{2} D_a(m_{R_n} - v^2, m_{R_n} - v^2).$$

A family of test functions φ_{R_n} is now constructed to satisfy: for large R_n

$$I_a^{\text{TFW}}(m_{R_n}) \leq E_a^{\text{TFW}}(\varphi_{R_n}, m_{R_n}) < E_a^{\text{TFW}}(0, m_{R_n}) = \frac{1}{2} D_a(m_{R_n}, m_{R_n}). \tag{5.45}$$

It follows from (5.45) that

$$I_a^{\text{TFW}}(m_{R_n}) = E_a^{\text{TFW}}(u_{a,R_n}, m_{R_n}) < E_a^{\text{TFW}}(0, m_{R_n}), \tag{5.46}$$

which implies that $u_{a,R_n} \not\equiv 0$, hence by the Harnack inequality $u_{a,R_n} > 0$ on $\mathbb{R}^3$ [12], hence (5.44) holds.

Let $\psi_{R_n} \in C_c^\infty(B_{4R_n}(0))$ satisfy $\psi_{R_n} \geq 0$ and $\psi_{R_n} = 1$ on $B_{2R_n}(0)$. Then let $\varepsilon > 0$ and consider the difference

$$E_a^{\text{TFW}}(\varepsilon \psi_{R_n}, m_{R_n}) - E_a^{\text{TFW}}(0, m_{R_n})$$
$$= \varepsilon^2 \left(\int |\nabla \psi_{R_n}|^2 - D_a(m_{R_n}, \psi_{R_n}^2) \right) + \frac{\varepsilon^4}{2} D_a(\psi_{R_n}^2, \psi_{R_n}^2) + \varepsilon^{10/3} \int \psi_{R_n}^{10/3}. \tag{5.47}$$

Applying (5.1) of Lemma 5.1, there exists $R_0 > 0$ such that for any $R_n \geq R_0$

$$\int_{\mathbb{R}^3} |\nabla \psi_{R_n}|^2 - D_a(m_{R_n}, \psi_{R_n}^2) \leq -C_0 R_n^3. \tag{5.48}$$

The remaining terms in (5.47) can be estimated for $0 < \varepsilon \leq 1$, using Young's inequality for convolutions and Cauchy-Schwarz, by

$$\frac{\varepsilon^4}{2} D_a(\psi_{R_n}^2, \psi_{R_n}^2) + \varepsilon^4 \int \psi_{R_n}^{10/3} \leq \frac{\varepsilon^4}{2} D_a(\chi_{B_{2R_n}(0)}, \chi_{B_{2R_n}(0)}) + \varepsilon^4 \int_{B_{2R_n}(0)} 1$$
$$\leq \left(\frac{1}{2} \|Y_a\|_{L^1(\mathbb{R}^3)} \|\chi_{B_{2R_n}(0)}\|_{L^2(\mathbb{R}^3)}^2 + \|\chi_{B_{2R_n}(0)}\|_{L^1(\mathbb{R}^3)} \right) \varepsilon^4$$
$$\leq C(1 + a^{-2}) R_n^3 \varepsilon^4 =: C_3 \varepsilon^4 R_n^3. \tag{5.49}$$

Combining the estimates (5.48)–(5.49) and choosing $0 < \varepsilon \le \varepsilon_0 := \min\{1, (\frac{C_0}{2C_3})^{1/2}\}$ ensures that

$$E_a^{\mathrm{TFW}}(\varepsilon\psi_{R_n}, m_{R_n}) - E_a^{\mathrm{TFW}}(0, m_{R_n}) \le \left(-C_0 + C_3\varepsilon^2\right)\varepsilon^2 R_n^3 < 0,$$

hence the desired estimate (5.45) holds. $\square$

Proof of Proposition 3.2. First suppose that $\mathrm{spt}(m)$ is bounded, then by Proposition 5.2 there exists $a_0 > 0$ such that for all $0 < a \le a_0$ and sufficiently large R_n, $m = m_{R_n}$ and hence $(u_a, \phi_a) = (u_{a,R_n}, \phi_{a,R_n})$ solves (2.3) and satisfies the desired estimate (3.3).

Now suppose $\mathrm{spt}(m)$ is unbounded, then the estimates (5.9)–(5.10) of Proposition 5.2 guarantee that for all $0 < a \le a_0$ and R_n sufficiently large, the sequences u_{a,R_n}, ϕ_{a,R_n} are bounded uniformly in $H^2_{\mathrm{unif}}(\mathbb{R}^3)$. Consequently, there exist $u_a, \phi_a \in H^2_{\mathrm{unif}}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ such that along a subsequence u_{a,R_n}, ϕ_{a,R_n} converges to u_a, ϕ_a, weakly in $H^2(B_R(0))$, strongly in $H^1(B_R(0))$ for all $R > 0$ and pointwise almost everywhere. It follows from the pointwise convergence that $u_a \ge 0$ and

$$\|u_a\|_{L^\infty(\mathbb{R}^3)} + \|\phi_a\|_{L^\infty(\mathbb{R}^3)} \le C(M).$$

Passing to the limit of the equations (5.8) in distribution shows the limit (u_a, ϕ_a) solves

$$-\Delta u_a + \frac{5}{3}u_a^{7/3} - \phi_a u_a = 0,$$
$$-\Delta\phi_a + a^2\phi_a = 4\pi(m - u_a^2).$$

Following the argument used to prove (5.9)–(5.10) in this instance yields the desired estimate (3.3) holds

$$\|u_a\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_a\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \le C(M).$$ $\square$

Proof of Proposition 3.1. This holds from applying Proposition 5.3 and following the proof of Proposition 3.2 in the unbounded case verbatim. $\square$

Proposition 5.4. *There exists $a_{\mathrm{c}} = a_{\mathrm{c}}(M, \omega) > 0$ and $c_{a_{\mathrm{c}}, M, \omega} > 0$ such that for all $m \in \mathcal{M}_{L^2}(M, \omega)$ and $0 < a \le a_{\mathrm{c}}$ the corresponding Yukawa ground state (u_a, ϕ_a) is unique and the electron density u_a satisfies*

$$\inf_{x\in\mathbb{R}^3} u_a(x) \ge c_{a_{\mathrm{c}}, M, \omega} > 0. \tag{5.50}$$

Proof of Proposition 5.4. The proof of Proposition 5.4 closely follows the proof of [11, Proposition 6.2] and [6, Theorem 6.10]. The estimate (5.50) is shown by contradiction, so suppose that for any $a_{\mathrm{c}} > 0$

$$\inf_{0 < a \le a_{\mathrm{c}}} \inf_{m\in\mathcal{M}_{L^2}(M,\omega)} \inf_{x\in\mathbb{R}^3} u_a(x) = 0,$$

hence there exists sequences $a_n \downarrow 0$ satisfying $a_n \le a_1$ for all $n \in \mathbb{N}$, $(m_n) \subset \mathcal{M}_{L^2}(M, \omega)$ and $(x_n) \subset \mathbb{R}^3$ such that for all $n \in \mathbb{N}$ the ground state (u_n, ϕ_n), corresponding to m_n with Yukawa parameter a_n, satisfies

$$u_n(x_n) \le \frac{1}{n}. \tag{5.51}$$

As $\frac{5}{3}u_n^{4/3} - \phi_n u_n \in L^2_{\mathrm{loc}}(\mathbb{R}^3)$, $u_n \in H^1_{\mathrm{unif}}(\mathbb{R}^3)$ and $u_n > 0$ solves

$$L_n u_n := \left(-\Delta + \frac{5}{3}u_n^{4/3} - \phi_n\right)u_n = 0,$$

applying the Harnack inequality [19], and observing that the coefficients of L_n are uniformly estimated by Proposition 3.1, this yields a uniform Harnack constant, hence for all $R > 0$, there exists $C = C(R, a_1, M) > 0$ such that for all $n \in \mathbb{N}$

$$\sup_{x \in B_R(x_n)} u_n(x) \leq C \inf_{x \in B_R(x_n)} u_n(x) \leq \frac{C}{n}.$$

It follows that the sequence of functions $u_n(\cdot + x_n)$ converges uniformly to zero on compact sets. Consider the ground state (u_n, ϕ_n) corresponding to the nuclear distribution m_n.

By the Harnack inequality, it follows that $u_n(\cdot + x_n)$ converges uniformly to 0 on compact subsets. Recall that ϕ_n satisfies

$$-\Delta \phi_n + a_n^2 \phi_n = 4\pi(m_n - u_n^2)$$

in distribution. In addition, ϕ_n and m_n satisfy

$$\|m_n(\cdot + x_n)\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_n(\cdot + x_n)\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(a_1, M).$$

It follows that along a subsequence $\phi_n(\cdot + x_n)$ converges to $\widetilde{\phi}$, weakly in $H^2(B_R(0))$, strongly in $H^1(B_R(0))$ for all $R > 0$ and pointwise almost everywhere. Also, $m_n(\cdot + x_n)$ converges to $\widetilde{m}$, weakly in $L^2(B_R(0))$ for all $R > 0$. By the Lebesgue-Besicovitch Differentiation Theorem [10], $\widetilde{m} \in \mathcal{M}_{L^2}(M, \omega)$. As $a_n \downarrow 0$, passing to the limit of

$$-\Delta \phi_n(\cdot + x_n) + a_n^2 \phi_n(\cdot + x_n) = 4\pi \left(m_n(\cdot + x_n) - u_n^2(\cdot + x_n) \right)$$

shows that $\widetilde{\phi}$ is a distributional solution of

$$-\Delta \widetilde{\phi} = 4\pi \widetilde{m}. \tag{5.52}$$

The argument of [6, Theorem 6.10] is now used to show that for all $R > 0$

$$\int_{B_R(0)} \widetilde{m}(z) \, \mathrm{d}z \leq CR. \tag{5.53}$$

As $\widetilde{m} \in \mathcal{M}_{L^2}(M, \omega)$, this leads to the contradiction that for all $R > 0$

$$\omega_0 R^3 - \omega_1 \leq \int_{B_R(0)} \widetilde{m}(z) \, \mathrm{d}z \leq CR.$$

To show (5.53) choose $\varphi \in C_c^\infty(B_2(0))$ such that $0 \leq \varphi \leq 1$ and $\varphi = 1$ on $B_1(0)$. Let $R > 0$, then testing (5.52) with $\varphi(\cdot/R)$ gives

$$-\frac{1}{R^2} \int_{B_{2R}(0)} \widetilde{\phi}(z)(\Delta\varphi)(z/R) \, \mathrm{d}z = 4\pi \int_{B_{2R}(0)} \widetilde{m}(z)\varphi(z/R) \, \mathrm{d}z. \tag{5.54}$$

The left-hand side can be estimated by

$$\frac{1}{R^2} \left| \int_{B_{2R}(0)} \widetilde{\phi}(z)(\Delta\varphi)(z/R) \, \mathrm{d}z \right| \leq \|\widetilde{\phi}\|_{L^\infty(\mathbb{R}^3)} \|\Delta\varphi\|_{L^\infty} \frac{|B_{2R}(0)|}{R^2} \leq CR, \tag{5.55}$$

where the constant $C > 0$ is independent of R. As $\widetilde{m} \geq 0$, combining (5.54)–(5.55) yields (5.53)

$$\int_{B_R(0)} \widetilde{m}(z) \, \mathrm{d}z \leq \int_{B_{2R}(0)} \widetilde{m}(z)\varphi(z/R) \, \mathrm{d}z \leq CR.$$

The contradiction ensures that there exists $a_c > 0$ and $c_{a_c, M, \omega} > 0$ such that for all $m \in \mathcal{M}_{L^2}(M, \omega)$ and $0 < a \leq a_c$, the corresponding Yukawa electron density u_a satisfies

$$\inf_{x \in \mathbb{R}^3} u_a(x) \geq c_{a_c, M, \omega} > 0. \qquad \square$$

Consequently, for $0 < a \leq a_c$, the electron density satisfies $\inf u_a > 0$, hence the arguments of [6, Chapter 6] can be applied verbatim to guarantee the uniqueness of the ground state (u_a, ϕ_a).

Remark 5. Theorem 3.5 provides an additional proof of Proposition 5.4. Let $a_0 > 0$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, then for any $0 < a \leq a_0$, [11, Propositions 3.1 and 3.2] and Proposition 3.1 guarantees that there exist corresponding Coulomb and Yukawa ground states (u, ϕ), (u_a, ϕ_a), respectively satisfying $\inf u \geq c_{M,\omega} > 0$ and $u_a \geq 0$. Then applying (3.6) of Theorem 3.5 implies

$$u_a(x) \geq u(x) - \|u_a - u\|_{L^\infty(\mathbb{R}^3)} \geq c_{M,\omega} - C'a^2,$$

hence for all $0 < a \leq a_c := \min\{a_0, (\frac{c_{M,\omega}}{2C'})^{1/2}\}$

$$\inf_{x \in \mathbb{R}^3} u_a(x) \geq c_{M,\omega} - C'a^2 \geq \frac{1}{2}c_{M,\omega} > 0.$$

$\square$

The proof of Proposition 3.3 requires the following result, which extends the lower bound on u_a from $0 < a \leq a_c$ to arbitrary $a > 0$.

Proposition 5.5. *Let $a_0 > a_c > 0$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, then for all $0 < a \leq a_0$ the corresponding Yukawa ground state (u_a, ϕ_a) is unique and there exists $c_{a_0,M,\omega} > 0$ such that the electron density u_a satisfies*

$$\inf_{x \in \mathbb{R}^3} u_a(x) \geq c_{a_0,M,\omega} > 0. \tag{5.56}$$

Due to the length of the argument, the proof of Proposition 5.5 is postponed to the Appendix, which can be found on Page 30.

Proof of Proposition 3.3. Combining Proposition 5.4 and Proposition 5.5 yields the desired result. $\square$

Proof of Corollary 3.4. This is identical to the proof of [11, Corollary 6.3], using the estimates (5.9)-(5.10) to provide the initial regularity. $\square$

5.2. **Proof of main results.** The proofs of Theorems 3.5, 3.7 and 3.8 closely follow the proofs of [11, Theorems 3.4 and 3.5], which adapts the uniqueness of the TFW equations [6, 3].

First, two alternative sets of assumptions on nuclear distributions m_1, m_2 are given. In the following, (u_0, ϕ_0) denotes the corresponding Coulomb ground state solving (2.2), i.e the ground state with Yukawa parameter $a = 0$.

(A) Let $k = 0$, $m_1 \in \mathcal{M}_{L^2}(M, \omega)$, $m_2 : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ satisfy

$$\|m_2\|_{L^2_{\text{unif}}(\mathbb{R}^3)} \leq M',$$

then by Proposition 3.2 there exist $a' = a'(\omega, m_2) > 0$ such that for all $0 \leq a_1 \leq a_2 \leq a'$ there exists $(u_1, \phi_1) = (u_{1,a_1}, \phi_{1,a_1})$ $(u_2, \phi_2) = (u_{2,a_2}, \phi_{2,a_2})$ solving either (2.2) or (2.3) corresponding to m_2, satisfying $\inf u_1 > 0$, $u_2 \geq 0$ and

$$\|u_2\|_{H^4_{\text{unif}}(\mathbb{R}^3)} + \|\phi_2\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \leq C(M'). \tag{5.57}$$

In addition, assume either $m_2 \not\equiv 0$ and $u_2 > 0$ or $m_2 = u_2 = \phi_2 = 0$.

Observe that (A) assumes that $u_2 > 0$, while Theorems 3.5 (with $k = 0$) and 3.7 only require either $u_a \geq 0$ or $u_{2,a} \geq 0$. The restriction $u_2 > 0$ will be lifted via a thermodynamic limit argument in the third part of its proof on page 26.

(B) Let $a_0 > 0$, $k \in \mathbb{N}_0$, $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$, $0 \leq a_1 \leq a_2 \leq a_0$ and let $(u_1, \phi_1) = (u_{1,a_1}, \phi_{1,a_1})$, $(u_2, \phi_2) = (u_{2,a_2}, \phi_{2,a_2})$ denote the corresponding ground states. (Note that (B) implies (A), with $a' = a_0$ and $M' = C(a_0, M)$.)

In addition, for both (A) and (B), define
$$w = u_1 - u_2, \quad \psi = \phi_1 - \phi_2,$$
and suppose that there exists $R \in H_{\text{unif}}^{k'}(\mathbb{R}^3)$, where $k' \in \{k, k+2\}$, such that (w, ψ) solves

$$-\Delta w + \frac{5}{3}\left(u_1^{7/3} - u_2^{7/3}\right) - \phi_1 u_1 + \phi_2 u_2 = 0, \tag{5.58a}$$

$$-\Delta \psi + a_1^2 \psi = 4\pi\left(u_2^2 - u_1^2\right) + R. \tag{5.58b}$$

Lemma 5.6. *Suppose that either* (A) *or* (B) *holds, then there exist* $C = C_A(M, M', \omega)$, $\gamma = \gamma_A(M, M', \omega) > 0$ *or* $C = C_B(a_0, k', M, \omega)$, $\gamma = \gamma_B(a_0, M, \omega) > 0$, *independent of both* a_1, a_2, *such that for any* $\xi \in H_\gamma$

$$\int_{\mathbb{R}^3}\left(\sum_{|\alpha_1|\leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2|\leq k'+2} |\partial^{\alpha_2}\psi|^2\right)\xi^2 \leq C\int_{\mathbb{R}^3}\sum_{|\beta|\leq k'} |\partial^\beta R|^2\xi^2. \tag{5.59}$$

In particular, for any $y \in \mathbb{R}^3$,

$$\sum_{|\alpha_1|\leq k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2|\leq k'} |\partial^{\alpha_2}\psi(y)|^2 \leq C\int_{\mathbb{R}^3}\sum_{|\beta|\leq k'} |\partial^\beta R(x)|^2 e^{-2\gamma|x-y|}\,\mathrm{d}x. \tag{5.60}$$

Further, if both $a_1 = a_2 = 0$, *then* $C = C_B(k', M, \omega)$, $\gamma = \gamma_B(M, \omega)$.

One of the key steps in proving Lemma 5.6 is showing

$$\int_{\mathbb{R}^3} \psi^2 \xi^2 \leq C\left(\int_{\mathbb{R}^3} R\psi\xi^2 + \int_{\mathbb{R}^3} (w^2 + \psi^2)|\nabla\xi|^2\right), \tag{5.61}$$

where the constant C is independent of a_1, a_2. However, due to the presence of the additional term in (5.58b), the argument in [11, Lemma 6.4] directly yields

$$a_1^2\int_{\mathbb{R}^3} \psi^2 \xi^2 \leq C\left(\int_{\mathbb{R}^3} R\psi\xi^2 + \int_{\mathbb{R}^3} (w^2 + \psi^2)|\nabla\xi|^2\right), \tag{5.62}$$

where the left-hand constant tends to 0 as $a_1 \to 0$. Instead, (5.61) is obtained by closely following the proof in the Coulomb setting.

In the following proof, all integrals are taken over $\mathbb{R}^3$.

Proof of Lemma 5.6. The argument closely follows the proof of [11, Lemma 6.7]. This proof describes the key steps of the argument and additional details are provided in [11].

Case 1. Suppose (B) holds, so $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$, so by Corollary 3.4 (or [11, Corollary 3.3] if either $a_i = 0$) for $i \in \{1, 2\}$

$$\|u_i\|_{H_{\text{unif}}^{k+4}(\mathbb{R}^3)} + \|\phi_i\|_{H_{\text{unif}}^{k+2}(\mathbb{R}^3)} \leq C(a_0, k, M, \omega)$$

and by Proposition 5.4 $\inf u_1, \inf u_2 \geq c_{a_c, M, \omega} > 0$ (if for $i \in \{1, 2\}$ $a_i = 0$ then by [11, Proposition 3.2] $\inf u_i \geq c_{M, \omega} > 0$). Let $\xi \in H^1(\mathbb{R}^3)$, then testing (5.58a) with $w\xi^2$ and re-arranging yields

$$\int |\nabla(w\xi)|^2 + \frac{5}{6}\int (u_1^{4/3} + u_2^{4/3})w^2\xi^2 - \frac{1}{2}\int (\phi_1 + \phi_2)w^2\xi^2 + \nu\int w^2\xi^2$$

$$\leq \int w^2|\nabla\xi|^2 + \frac{1}{2}\int \psi(u_1^2 - u_2^2)\xi^2, \tag{5.63}$$

where $\nu = \frac{1}{2}(u_1^{4/3} + u_2^{4/3}) \geq \frac{1}{2}c_{ac,M,\omega}^{4/3} > 0$ (or $\nu \geq \frac{1}{2}c_{M,\omega}^{4/3} > 0$ when $a_1 = a_2 = 0$). As $u_1, u_2 > 0$, [11, Lemma 6.2] implies that

$$L = -\Delta + \tfrac{5}{6}(u_1^{4/3} + u_2^{4/3}) - \tfrac{1}{2}(\phi_1 + \phi_2)$$

is a non-negative operator, hence (5.63) can be expressed as

$$\langle w\xi, L(w\xi)\rangle + \nu \int w^2\xi^2 \leq \int w^2|\nabla\xi|^2 + \frac{1}{2}\int \psi(u_1^2 - u_2^2)\xi^2, \tag{5.64}$$

Then, testing (5.58b) with $\psi\xi^2$ and re-arranging and using $a_1 \geq 0$ gives

$$\int |\nabla(\psi\xi)|^2 \leq \int |\nabla(\psi\xi)|^2 + a_1^2 \int \psi^2\xi^2 \leq \int R\psi\xi^2 + 4\pi\int \psi(u_2^2 - u_1^2)\xi^2. \tag{5.65}$$

Combining (5.64) and (5.65) and further re-arrangement yields

$$\langle w\xi, L(w\xi)\rangle + \nu \int w^2\xi^2 + \frac{1}{8\pi}\int |\nabla\psi|^2\xi^2 \leq C\left(\int R\psi\xi^2 + \int (w^2 + \psi^2)|\nabla\xi|^2\right). \tag{5.66}$$

From this point, the proof of [11, Lemma 6.7] follows verbatim to show the estimate: there exists $C, \gamma > 0$ such that for all $\xi \in H_\gamma$

$$\int_{\mathbb{R}^3}\left(\sum_{|\alpha_1|\leq k+4}|\partial^{\alpha_1}w|^2 + \sum_{|\alpha_2|\leq k+2}|\partial^{\alpha_2}\psi|^2\right)\xi^2 \leq C\int_{\mathbb{R}^3}\sum_{|\beta|\leq k}|\partial^\beta R|^2\xi^2. \tag{5.67}$$

If $k' = k$, then this is the desired estimate (5.59). Alternatively, if $k' = k+2$, the remaining estimate is shown by adapting the proof of [11, Lemma 6.6]. Recall (5.58b), that ψ solves

$$-\Delta\psi = -a_1^2\psi + 4\pi\left(u_2^2 - u_1^2\right) + R \in H_{\text{unif}}^{k+2}(\mathbb{R}^3), \tag{5.68}$$

hence by standard elliptic regularity [9] $\psi \in H_{\text{unif}}^{k+4}(\mathbb{R}^3)$. It follows that

$$\int \sum_{|\alpha|\leq k+2}|\partial^\alpha\Delta\psi|^2\xi^2 \leq C(k',M,\omega)\int \sum_{|\beta|\leq k+2}\left(|\partial^\beta\psi|^2 + |\partial^\beta R|^2 + |\partial^\beta w|^2\right)\xi^2. \tag{5.69}$$

In addition, applying integration by parts, for any $k_1 \leq k+2$

$$\sum_{|\alpha|=k_1+2}\int |\partial^\alpha\psi|^2\xi^2 \leq C\left(\int \sum_{|\beta_1|=k_1}|\partial^{\beta_1}\Delta\psi|^2\xi^2 + \int \sum_{|\beta_2|=k_1+1}|\partial^{\beta_2}\psi|^2\xi^2\right), \tag{5.70}$$

hence combining (5.67)–(5.70) for $k_1 = k+2$ gives

$$\begin{aligned}
\sum_{|\alpha|=k+4}\int |\partial^\alpha\psi|^2\xi^2 &\leq C\left(\int \sum_{|\beta_1|=k+2}|\partial^{\beta_1}\Delta\psi|^2\xi^2 + \int \sum_{|\beta_2|=k+3}|\partial^{\beta_2}\psi|^2\xi^2\right) \\
&\leq C\left(\int \sum_{|\beta_1|=k+2}|\partial^{\beta_1}\Delta\psi|^2\xi^2 + \int \sum_{|\beta_2|=k+2}|\partial^{\beta_2}\psi|^2\xi^2\right) \\
&\leq C\int \sum_{|\beta|\leq k+2}\left(|\partial^\beta\psi|^2 + |\partial^\beta R|^2 + |\partial^\beta w|^2\right)\xi^2 \\
&\leq C\int_{\mathbb{R}^3}\sum_{|\beta|\leq k+2}|\partial^\beta R|^2\xi^2. \tag{5.71}
\end{aligned}$$

Inserting (5.71) into (5.67) yields the desired estimate (5.59)

$$\int_{\mathbb{R}^3}\left(\sum_{|\alpha_1|\leq k+4}|\partial^{\alpha_1}w|^2 + \sum_{|\alpha_2|\leq k'}|\partial^{\alpha_2}\psi|^2\right)\xi^2 \leq C\int_{\mathbb{R}^3}\sum_{|\beta|\leq k'}|\partial^\beta R|^2\xi^2.$$

Let $y \in \mathbb{R}^3$, then applying (5.67) with $\xi(x) = e^{-\gamma|x-y|} \in H_\gamma$ and following the proof of [11, Lemma 6.6] yields the remaining estimate (5.60).

Case 2. Suppose (A) holds, then by Proposition 5.2

$$\|u_1\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_1\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M),$$
$$\|u_2\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_2\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M'),$$

and $\inf u_1 \geq c_{a',M,\omega} > 0$ (if $a_1 = 0$ then $\inf u_1 \geq c_{M,\omega} > 0$) and $u_2 \geq 0$. Other than this, the argument of Case 1 holds verbatim to obtain (5.59)–(5.60). $\square$

Proof of Corollary 3.6. As $m \in \mathcal{M}_{H^k}(M,\omega)$, applying Lemma 5.6(B) with $0 < a_1 \leq a_2 \leq a_0$ and $R = (a_2^2 - a_1^2)\phi_2 \in H^{k+2}_{\mathrm{unif}}(\mathbb{R}^3)$. Then applying Lemma 5.6 case (B) with $\xi(x) = e^{-\gamma|x-y|} \in H_\gamma$ yields

$$\sum_{|\alpha|\leq k+2} \left(|\partial^\alpha w(y)|^2 + |\partial^\alpha \psi(y)|^2\right) \leq C(a_2^2 - a_1^2) \int_{\mathbb{R}^3} \sum_{|\beta|\leq k+2} |\partial^\beta \phi_2(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x.$$

As $\phi_2 \in H^{k+2}_{\mathrm{unif}}(\mathbb{R}^3)$, and for all $z \in \mathbb{R}^3$ and $A \subset B_1(z)$, $\sup_{x\in A} e^{-2\gamma|x|} \leq C \inf_{x\in A} e^{-2\gamma|x|}$, it follows that

$$\sum_{|\alpha|\leq k+2} \left(|\partial^\alpha w(y)|^2 + |\partial^\alpha \psi(y)|^2\right) \leq C(a_2^2 - a_1^2) \int_{\mathbb{R}^3} \sum_{|\beta|\leq k+2} |\partial^\beta \phi_2(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x$$
$$\leq C(a_2^2 - a_1^2)\|\phi_2\|^2_{H^{k+2}_{\mathrm{unif}}(\mathbb{R}^3)} \int_{\mathbb{R}^3} e^{-2\gamma|x-y|} \, \mathrm{d}x \leq C(a_2^2 - a_1^2),$$

where the final constant is independent of $y \in \mathbb{R}^3$, hence the desired estimate (3.7) holds. $\square$

Proof of Theorem 3.5. For $0 < a \leq a_0$, applying Corollary 3.6 with $a_1 = 0, a_2 = a$ yields the desired estimate (3.6). $\square$

Proof of Theorem 3.8. Let $0 < a \leq a_0$, then as $m_1, m_2 \in \mathcal{M}_{H^k}(M,\omega)$ for $k \in \mathbb{N}_0$, applying Lemma 5.6(B) with $a_1 = a_2 = a$ and $R = 4\pi(m_1 - m_2) \in H^k_{\mathrm{unif}}(\mathbb{R}^3)$ yields the desired estimate (3.12). $\square$

Proof of Theorem 3.7. The proof closely follows and adapts the argument used to show [11, Theorem 3.4].

As $m_1 \in \mathcal{M}_{L^2}(M,\omega)$, by Proposition 3.3 for all $a > 0$ there exists a unique ground state $(u_{1,a}, \phi_{1,a})$ corresponding to m_1. It remains to show that m_2 and its corresponding solution satisfy the conditions of Lemma 5.6(A).

Case 1. Suppose $\mathrm{spt}(m_2)$ is bounded and $m_2 \not\equiv 0$. Since $m_2 \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$, it follows that $m_2 \in L^1(\mathbb{R}^3)$ and since $m_2 \geq 0$ and $m_2 \not\equiv 0$, it follows that $\int m_2 > 0$. For $a > 0$, consider the minimisation problem

$$I_a^{\mathrm{TFW}}(m_2) = \inf \left\{ E_a^{\mathrm{TFW}}(v, m_2) \,\middle|\, v \in H^1(\mathbb{R}^3), v \geq 0 \right\}.$$

By Proposition 5.2, there exists $a_0 = a_0(m_2) > 0$ such that for all $0 < a \leq a_0$, the minimisation problem yields a unique solution $(u_{2,a}, \phi_{2,a})$ of (2.3), satisfying $u_{2,a} > 0$ and (3.9)

$$\|u_{2,a}\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_{2,a}\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M'),$$

independently of a. Consequently, applying Lemma 5.6(A) with $0 < a_1 = a_2 \leq a' \leq 1$ and $R = 4\pi(m_1 - m_2) \in H^k_{\mathrm{unif}}(\mathbb{R}^3)$ yields the desired estimate (3.10).

Case 2. Suppose $m_2 = u_2 = \phi_2 = 0$, then by definition (u_2, ϕ_2) solve (2.2) and (A) is satisfied, so applying Lemma 5.6(A) with $0 < a_1 = a_2 \leq a' = 1$ and $R = 4\pi(m_1 - m_2) \in H_{\text{unif}}^k(\mathbb{R}^3)$ yields the desired estimate (3.10).

Case 3. Suppose $\text{spt}(m_2)$ is unbounded. By Proposition 5.2, there exists $a_0 = a_0(m_2) > 0$ such that for all $0 < a \leq a_0$, there exists $(u_{2,a}, \phi_{2,a})$ solving (2.3) and satisfying $u_{2,a} \geq 0$. As it is not guaranteed that $u_{2,a} > 0$, it is not possible to apply Lemma 5.6(A) directly to compare $(u_{1,a}, \phi_{1,a})$ with $(u_{2,a}, \phi_{2,a})$. Instead, by following the proof of Proposition 5.2, a thermodynamic limit argument is used to construct a sequence of functions $(u_{2,a,R_n}, \phi_{2,a,R_n})$ which satisfy (A) for sufficiently large R_n and converge to $(u_{2,a}, \phi_{2,a})$ as $R_n \to \infty$.

Let $R_n \uparrow \infty$ and define $m_{2,R_n} := m_2 \cdot \chi_{B_{R_n}(0)}$, then as $m_2 \in L_{\text{unif}}^2(\mathbb{R}^3)$, $m_2 \geq 0$ and $m_2 \not\equiv 0$, it follows that $m_{2,R_n} \in L^1(\mathbb{R}^3)$ and for sufficiently large R_n, $\int m_{2,R_n} > 0$. By Proposition 5.2, there exists $R_0 = R_0(m_2), a_0 = a_0(m_2) > 0$ such that for all $R_n \geq R_0$ and $0 < a \leq a_0$ the minimisation problem

$$I_a^{\text{TFW}}(m_{2,R_n}) = \inf \left\{ E_a^{\text{TFW}}(v, m_{2,R_n}) \,\middle|\, v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_{2,R_n} \right\},$$

defines a unique solution $(u_{2,a,R_n}, \phi_{2,a,R_n})$ to (2.3), satisfying $u_{2,a,R_n} > 0$ and

$$\|u_{2,a,R_n}\|_{H_{\text{unif}}^4(\mathbb{R}^3)} + \|\phi_{2,a,R_n}\|_{H_{\text{unif}}^2(\mathbb{R}^3)} \leq C(M'), \tag{5.72}$$

where the constant is independent of a, a_0 and R_n. Passing to the limit in (5.72), there exist $u_{2,a} \in H_{\text{unif}}^4(\mathbb{R}^3), \phi_{2,a} \in H_{\text{unif}}^2(\mathbb{R}^3)$ such that, respectively, along a subsequence $u_{2,a,R_n}, \phi_{2,a,R_n}$ converges to $u_{2,a}, \phi_{2,a}$, weakly in $H^4(B_R(0))$ and $H^2(B_R(0))$, strongly in $H^2(B_R(0))$ and $L^2(B_R(0))$ for all $R > 0$ and for all $|\alpha| \leq 2$, $\partial^\alpha u_{2,a,R_n}, \phi_{2,a,R_n}$ converges to $\partial^\alpha u_{2,a}, \phi_{2,a}$ pointwise. It follows that $(u_{2,a}, \phi_{2,a})$ is a solution of (2.3) corresponding to m_2, satisfying $u_{2,a} \geq 0$ and (3.9)

$$\|u_{2,a}\|_{H_{\text{unif}}^4(\mathbb{R}^3)} + \|\phi_{2,a}\|_{H_{\text{unif}}^2(\mathbb{R}^3)} \leq C(M').$$

In addition, for $0 < a \leq a' = a_0$, $(u_1', \phi_1') = (u_{1,a}, \phi_{1,a})$ and $(u_2', \phi_2') = (u_{2,a,R_n}, \phi_{2,a,R_n})$ satisfy (A) for all $R_n \geq R_0$, so by Lemma 5.6 that there exist $C, \gamma > 0$, independent of a, a_0 and R_n, such that for $R_n \geq R_0$ and any $\xi \in H_\gamma$

$$\int_{\mathbb{R}^3} \left(\sum_{|\alpha_1| \leq 4} |\partial^{\alpha_1}(u_{1,a} - u_{2,a,R_n})|^2 + \sum_{|\alpha_2| \leq 2} |\partial^{\alpha_2}(\phi_{1,a} - \phi_{2,a,R_n})|^2 \right) \xi^2$$

$$\leq C \int_{\mathbb{R}^3} (m_1 - m_{2,R_n})^2 \xi^2, \tag{5.73}$$

and for any $y \in \mathbb{R}^3$,

$$\sum_{|\alpha_1| \leq 2} |\partial^{\alpha_1}(u_{1,a} - u_{2,a,R_n})(y)|^2 + |(\phi_{1,a} - \phi_{2,a,R_n})(y)|^2$$

$$\leq C \int_{\mathbb{R}^3} |(m_1 - m_{2,R_n})(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x. \tag{5.74}$$

Using the pointwise convergence of $(u_{2,a,R_n}, \phi_{2,a,R_n})$ to $(u_{2,a}, \phi_{2,a})$, applying the Dominated Convergence Theorem and sending $R_n \to \infty$ in (5.73)–(5.74) gives the desired estimates (3.10)–(3.11). $\qquad\square$

5.3. **Proof of Applications.** Proving Theorem 4.1 first requires establishing the existence, uniqueness and regularity of solutions to the linearised TFW Yukawa equations.

Fix $Y = (Y_j)_{j \in \mathbb{N}} \in \mathcal{Y}_{L^2}(M, \omega)$ and let $m = m_Y \in \mathcal{M}_{L^2}(M, \omega)$. Let $V \in \mathbb{R}^3 \smallsetminus \{0\}$, $k \in \mathbb{N}$ and for $h \in [0, 1]$ define

$$Y^h = \{ Y_j + \delta_{jk} hV \mid j \in \mathbb{N} \}, \tag{5.75}$$

and the associated nuclear configuration

$$m_h(x) = m(x) + \eta(x - Y_k - hV) - \eta(x - Y_k). \tag{5.76}$$

By [11, Lemma 6.7], there exist (M', ω') such that $m_h \in \mathcal{Y}_{L^2}(M', \omega')$ for all $h \in [0, 1]$, hence by Proposition 3.1 for all $a > 0$ there exists a corresponding ground state $(u_{a,h}, \phi_{a,h})$. Also, let $(u_a, \phi_a) = (u_{a,0}, \phi_{a,0})$. Corollary 4.3 is now used to compare $(u_{a,h}, \phi_{a,h})$ with (u_a, ϕ_a) to rigorously linearise the TFW Yukawa equations.

Lemma 5.7. *Let $a_0 > 0$, $Y \in \mathcal{Y}_{L^2}(M, \omega)$ and let $m = m_Y \in \mathcal{M}_{L^2}(M, \omega)$. Also, let $k \in \mathbb{N}$, $V \in \mathbb{R}^3 \smallsetminus \{0\}$ and $h_0 = \min\{1, |V|^{-1}\}$. For $h \in [0, h_0]$ define*

$$m_h(x) = m(x) + \eta(x - Y_k - hV) - \eta(x - Y_k),$$

then for all $0 < a \le a_0$ and $h \in [0, h_0]$ there exists a unique Yukawa ground state $(u_{a,h}, \phi_{a,h})$ corresponding to m_h. There exist $C = C(a_0, M', \omega')$, $\gamma_0 = \gamma_0(a_0, M', \omega') > 0$, independent of a, h and $|V|$, such that for all $0 < a \le a_0$ and $h \in [0, h_0]$

$$\sum_{|\alpha| \le 2} \left(|\partial^\alpha (u_{a,h} - u_a)(x)| + |\partial^\alpha (\phi_{a,h} - \phi_a)(x)| \right) + |(m_h - m)(x)| \le Che^{-\gamma|x - Y_k|}, \tag{5.77}$$

$$\|u_{a,h} - u_a\|_{H^4(\mathbb{R}^3)} + \|\phi_{a,h} - \phi_a\|_{H^2(\mathbb{R}^3)} \le C\|m_h - m\|_{L^2(\mathbb{R}^3)} \le Ch. \tag{5.78}$$

Moreover, for all $0 < a \le a_0$, the limits

$$\overline{u}_a = \lim_{h \to 0} \frac{u_{a,h} - u_a}{h}, \quad \overline{\phi}_a = \lim_{h \to 0} \frac{\phi_{a,h} - \phi_a}{h}, \quad \overline{m} = \lim_{h \to 0} \frac{m_h - m}{h},$$

exist and $(\overline{u}_a, \overline{\phi}_a)$ is the unique solution to the linearised TFW Yukawa equations

$$- \Delta \overline{u}_a + \left(\frac{35}{9} u_a^{4/3} - \phi_a \right) \overline{u}_a - u_a \overline{\phi}_a = 0, \tag{5.79a}$$

$$- \Delta \overline{\phi}_a + a^2 \overline{\phi}_a = 4\pi \left(\overline{m} - 2u_a \overline{u}_a \right). \tag{5.79b}$$

Moreover, $\overline{u}_a \in H^4(\mathbb{R}^3), \overline{\phi}_a \in H^2(\mathbb{R}^3), \overline{m} \in C_c^\infty(\mathbb{R}^3)$ and satisfy

$$\sum_{|\alpha| \le 2} \left(|\partial^\alpha \overline{u}_a(x)| + |\partial^\alpha \overline{\phi}_a(x)| \right) + |\overline{m}(x)| \le Ce^{-\gamma|x - Y_k|}, \tag{5.80}$$

$$\|\overline{u}_a\|_{H^4(\mathbb{R}^3)} + \|\overline{\phi}_a\|_{H^2(\mathbb{R}^3)} \le C\|\overline{m}\|_{L^2(\mathbb{R}^3)}, \tag{5.81}$$

where $C = C(a_0, M', \omega')$, $\gamma_0 = \gamma_0(a_0, M', \omega') > 0$ are independent of a and $|V|$.

Proof of Lemma 5.7. The first step is to show the uniqueness of the linearised Yukawa solution $(\overline{u}_a, \overline{\phi}_a)$ to (5.79). Let $0 < a \le a_0$ and suppose $(w, \psi) \in H^1(\mathbb{R}^3) \times H^1(\mathbb{R}^3)$ solves

$$- \Delta w + \left(\frac{35}{9} u_a^{4/3} - \phi_a \right) w - u_a \psi = 0, \tag{5.82a}$$

$$- \Delta \psi + a^2 \psi = -8\pi u_a \psi. \tag{5.82b}$$

Testing (5.82a) with w yields

$$\int_{\mathbb{R}^3} |\nabla w|^2 + \int_{\mathbb{R}^3} \left(\frac{35}{9} u_a^{4/3} - \phi_a \right) w^2 = \int_{\mathbb{R}^3} u_a w \psi.$$

Then as $u_a > 0$, by [11, Lemma 6.2] $L_a = -\Delta + \frac{35}{9}u_a^{4/3} - \phi_a$ is a non-negative operator. In addition, by Proposition 3.3 $\inf u_a \geq c_{a_0,M',\omega'} > 0$, hence there exists $c_0 > 0$ such that

$$c_0 \int_{\mathbb{R}^3} w^2 \leq \frac{10}{9} \int_{\mathbb{R}^3} u_a^{4/3} w^2 \leq \langle w, L_a w \rangle + \frac{10}{9} \int_{\mathbb{R}^3} u_a^{4/3} w^2$$

$$= \int_{\mathbb{R}^3} |\nabla w|^2 + \int_{\mathbb{R}^3} \left(\frac{35}{9} u_a^{4/3} - \phi_a \right) w^2 = \int_{\mathbb{R}^3} u_a w \psi. \tag{5.83}$$

Then testing (5.82b) with $\frac{1}{8\pi}\psi$ gives

$$\frac{1}{8\pi} \left(\int_{\mathbb{R}^3} |\nabla \psi|^2 + a^2 \int_{\mathbb{R}^3} \psi^2 \right) = -\int_{\mathbb{R}^3} u_a w \psi, \tag{5.84}$$

and adding (5.83)–(5.84) yields

$$0 \leq c_0 \int_{\mathbb{R}^3} w^2 + \frac{1}{8\pi} \left(\int_{\mathbb{R}^3} |\nabla \psi|^2 + a^2 \int_{\mathbb{R}^3} \psi^2 \right) \leq 0,$$

hence $w = \psi = 0$ almost everywhere, so (5.79) has a unique solution in $H^1(\mathbb{R}^3) \times H^1(\mathbb{R}^3)$.

Now, Proposition 3.2 and Proposition 5.4 imply that for $0 < a \leq a_0$ and $h \in [0, h_0]$ the ground state $(u_{a,h}, \phi_{a,h})$ satisfies

$$\|u_{a,h}\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_{a,h}\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(a_0, M'), \tag{5.85}$$

$$\inf_{x \in \mathbb{R}^3} u_{a,h}(x) \geq c_{a_0,M',\omega'} > 0, \tag{5.86}$$

independently of a, h and $|V|$. Then following the proof of [11, Lemma 6.8], for all $0 < a \leq a_0$ and $h \in [0, h_0]$, the estimates (5.77)–(5.78) hold. In addition, there exist $\overline{u}_a \in H^4(\mathbb{R}^3)$ and $\overline{\phi}_a \in H^2(\mathbb{R}^3)$ such that along a subsequence h_n (which may depend on a) such that $\frac{u_{a,h_n} - u_a}{h_n}, \frac{\phi_{a,h_n} - \phi_a}{h_n}$ converge to $\overline{u}_a \in H^4(\mathbb{R}^3), \overline{\phi}_a \in H^2(\mathbb{R}^3)$ respectively, weakly in $H^4(\mathbb{R}^3)$ and $H^2(\mathbb{R}^3)$, strongly in $H^3(B_R(0))$ and $H^1(B_R(0))$ for all $R > 0$ and pointwise almost everywhere, along with their derivatives. In addition, it follows that $(\overline{u}_a, \overline{\phi}_a)$ satisfy (5.80)–(5.81).

To verify that $(\overline{u}_a, \overline{\phi}_a)$ are independent of the sequence chosen, passing to the limit in the equations

$$-\Delta \left(\frac{u_{a,h_n} - u_a}{h_n} \right) + \frac{5}{3} \frac{u_{a,h_n}^{7/3} - u_a^{7/3}}{h_n} - \frac{\phi_{a,h_n} u_{a,h_n} - \phi_a u_a}{h_n} = 0,$$

$$-\Delta \left(\frac{\phi_{a,h_n} - \phi_a}{h_n} \right) + a^2 \left(\frac{\phi_{a,h_n} - \phi_a}{h_n} \right) = 4\pi \left(\frac{m_{h_n} - m}{h_n} - \frac{u_{a,h_n}^2 - u_a^2}{h_n} \right),$$

gives that $(\overline{u}_a, \overline{\phi}_a)$ solve the linearised Yukawa equations (5.79) pointwise,

$$-\Delta \overline{u}_a + \left(\frac{35}{9} u_a^{4/3} - \phi_a \right) \overline{u}_a - u_a \overline{\phi}_a = 0,$$

$$-\Delta \overline{\phi}_a + a^2 \overline{\phi}_a = 4\pi \left(\overline{m} - 2u_a \overline{u}_a \right),$$

$$\text{where} \quad \overline{m}(x) = \lim_{h_n \to 0} \frac{(m_{h_n} - m)(x)}{h_n} = -\nabla \eta(x - Y_k) \cdot V.$$

Clearly $\overline{m}$ is independent of the sequence h_n, so as $(\overline{u}_a, \overline{\phi}_a)$ is the unique solution to the linearised Yukawa system (5.79), it is independent of the sequence (h_n). It then follows that $\frac{u_{a,h} - u_a}{h}, \frac{\phi_{a,h} - \phi_a}{h}$ converge to $\overline{u}_a, \overline{\phi}_a$ as $h \to 0$ as stated above. $\qquad \square$

Proof of Theorem 4.1. Let $0 < a \le a_0$ and $h \in [0, h_0]$, then recall (4.4)

$$\mathcal{E}_{2,a}(Y^h; \cdot) = |\nabla u_{a,h}|^2 + u_{a,h}^{10/3} + \tfrac{1}{8\pi} \left(|\nabla \phi_{a,h}|^2 + a^2 \phi_{a,h}^2 \right).$$

Applying Lemma 5.7 and using the pointwise convergence of $u_{a,h}, \phi_{a,h}, \frac{u_{a,h} - u_a}{h}, \frac{\phi_{a,h} - \phi_a}{h}$ to $u_a, \phi_a, \overline{u}_a, \overline{\phi}_a$ as $h \to 0$, along with their derivatives, it follows that

$$\frac{\mathcal{E}_{2,a}(Y^h; \cdot) - \mathcal{E}_{2,a}(Y; \cdot)}{h} \to 2\nabla u_a \cdot \nabla \overline{u}_a + \frac{10}{3} u_a^{7/3} \overline{u}_a + \frac{1}{4\pi} \left(\nabla \phi_a \cdot \nabla \overline{\phi}_a + a^2 \phi_a \overline{\phi}_a \right).$$

As $u_a \in W^{1,\infty}(\mathbb{R}^3)$, $\phi_a \in L^\infty(\mathbb{R}^3)$ and $\nabla \phi_a \in L^2_{\text{unif}}(\mathbb{R}^3)$ and (5.80) holds

$$\sum_{|\alpha| \le 2} \left(|\partial^\alpha \overline{u}_a(x)| + |\partial^\alpha \overline{\phi}_a(x)| \right) + |\overline{m}(x)| \le C e^{-\gamma_0 |x - Y_k|},$$

it follows that $\partial_{Y_k} \mathcal{E}_{2,a} \in L^1(\mathbb{R}^3)$ and

$$\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{2,a}(Y; x)}{\partial Y_k} \, \mathrm{d}x = 2 \int_{\mathbb{R}^3} \nabla u_a \cdot \nabla \overline{u}_a + \frac{10}{3} \int_{\mathbb{R}^3} u_a^{7/3} \overline{u}_a$$
$$+ \frac{1}{4\pi} \int_{\mathbb{R}^3} \left(\nabla \phi_a \cdot \nabla \overline{\phi}_a + a^2 \phi_a \overline{\phi}_a \right). \tag{5.87}$$

An identical argument shows that $\partial_{Y_k} \mathcal{E}_{1,a} \in L^1(\mathbb{R}^3)$ and

$$\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{1,a}(Y; x)}{\partial Y_k} \, \mathrm{d}x = 2 \int_{\mathbb{R}^3} \nabla u_a \cdot \nabla \overline{u}_a + \frac{10}{3} \int_{\mathbb{R}^3} u_a^{7/3} \overline{u}_a$$
$$+ \frac{1}{2} \int_{\mathbb{R}^3} \left(\phi_a(\overline{m} - 2u_a \overline{u}_a) + \overline{\phi}_a(m - u_a^2) \right). \tag{5.88}$$

Using that ϕ_a and $\overline{\phi}_a$ solve (2.3b) and (5.79b), respectively,

$$\frac{1}{2} \int_{\mathbb{R}^3} \overline{\phi}_a(m - u_a^2) = \frac{1}{8\pi} \int_{\mathbb{R}^3} \overline{\phi}_a(-\Delta \phi_a + a^2 \phi_a) = \frac{1}{8\pi} \int_{\mathbb{R}^3} \left(\nabla \phi_a \cdot \nabla \overline{\phi}_a + a^2 \phi_a \overline{\phi}_a \right)$$
$$= \frac{1}{8\pi} \int_{\mathbb{R}^3} \phi_a(-\Delta \overline{\phi}_a + a^2 \overline{\phi}_a) = \frac{1}{2} \int_{\mathbb{R}^3} \phi_a(\overline{m} - 2u_a \overline{u}_a). \tag{5.89}$$

Combining (5.87)–(5.89) and using that u_a solves (2.3a), $-\Delta u_a + \frac{5}{3} u_a^{7/3} - \phi_a u_a = 0$, the estimate (4.8) follows

$$\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{1,a}(Y; x)}{\partial Y_k} \, \mathrm{d}x = \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{2,a}(Y; x)}{\partial Y_k} \, \mathrm{d}x$$
$$= 2 \left(\int_{\mathbb{R}^3} \nabla u_a \cdot \nabla \overline{u}_a + \frac{5}{3} \int_{\mathbb{R}^3} u_a^{7/3} \overline{u}_a - \int_{\mathbb{R}^3} \phi_a u_a \overline{u}_a \right) + \int_{\mathbb{R}^3} \phi_a \overline{m} = \int_{\mathbb{R}^3} \phi_a \overline{m}.$$

Now recall the corresponding result for the Coulomb case [11, (4.21)], that $\partial_{Y_k} \mathcal{E}_1, \partial_{Y_k} \mathcal{E}_2 \in L^1(\mathbb{R}^3)$ and

$$\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_1(Y; x)}{\partial Y_k} \, \mathrm{d}x = \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_2(Y; x)}{\partial Y_k} \, \mathrm{d}x = \int_{\mathbb{R}^3} \phi \, \overline{m}.$$

Applying (3.6) of Theorem 3.5 and (5.80) of Lemma 5.7 yields the desired estimate (4.9), for $i \in \{1, 2\}$

$$\left| \int_{\mathbb{R}^3} \left(\frac{\partial \mathcal{E}_{i,a}}{\partial Y_k} - \frac{\partial \mathcal{E}_i}{\partial Y_k} \right) (Y; x) \, \mathrm{d}x \right|$$
$$\le \int_{\mathbb{R}^3} |\phi_a - \phi| |\overline{m}| \le C \|\phi_a - \phi\|_{L^\infty(\mathbb{R}^3)} \int_{\mathbb{R}^3} e^{-\gamma |x - Y_k|} \, \mathrm{d}x \le C a^2. \qquad \square$$

Proof of Proposition 4.2. This holds directly from applying Theorem 3.7 and following the proof of [11, Proposition 4.1] verbatim. □

Proof of Corollary 4.3. This holds directly from applying Theorem 3.8 and following the proof of [11, Corollary 4.2] verbatim. □

Proof of Corollary 4.4. This holds directly from applying Theorem 3.8 with $k = 0$ and following the proof of [11, Theorem 4.3] verbatim. □

6. APPENDIX

The purpose of this section is to prove Proposition 5.5.

Proposition 5.5. *Let $a_0 > a_c > 0$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, then for all $0 < a \leq a_0$ the corresponding Yukawa ground state (u_a, ϕ_a) is unique and there exists $c_{a_0, M, \omega} > 0$ such that the electron density u_a satisfies*

$$\inf_{x \in \mathbb{R}^3} u_a(x) \geq c_{a_0, M, \omega} > 0. \tag{5.56}$$

The proof of Proposition 5.5 adapts the argument described in [6, Remark 4.16, Lemma 4.14], which shows that the periodic Yukawa ground state is bounded below and hence unique. The proof requires the following result.

Lemma 6.1. *For any $a_0 > 0$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, there exists $R_0 = R_0(a_0, \omega)$, $\nu_{a_0, M, \omega} > 0$ such that for all $0 < a \leq a_0$ and $R_n \geq R_0$*

$$\inf_{x \in B_1(0)} u_{a, R_n}(x) \geq \nu_{a_0, M, \omega} > 0. \tag{6.1}$$

Then, sending $R_n \to \infty$ in (6.1), it follows that for all $0 < a \leq a_0$

$$\inf_{x \in B_1(0)} u_a(x) \geq \nu_{a_0, M, \omega} > 0,$$

hence $u_a > 0$. Then following the proof of [6, Lemma 4.14] gives the desired estimate (5.56). As the argument used in [6, Lemma 4.14] is also necessary to show Lemma 6.1, it is followed closely in this instance and for the proof of Proposition 5.5, only the necessary changes in the argument are described.

Proof of Lemma 6.1. It is first shown that there exists $R_0' > 0$ such that for all $0 < a \leq a_c$

$$\inf_{R_n \geq R_0'} \inf_{m \in \mathcal{M}_{L^2}(M, \omega)} \inf_{x \in B_1(0)} u_{a, R_n, m}(x) \geq \frac{c_{a_c, M, \omega}}{2} > 0, \tag{6.2}$$

then it remains to show that there exists $R_0 > 0$ such that for all $a_c < a \leq a_0$

$$\inf_{R_n \geq R_0} \inf_{m \in \mathcal{M}_{L^2}(M, \omega)} \inf_{x \in B_1(0)} u_{a, R_n, m}(x) = c_{a_0, M, \omega} > 0. \tag{6.3}$$

By Proposition 5.4, for any $m \in \mathcal{M}_{L^2}(M, \omega)$, $0 < a \leq a_c$, the Yukawa ground state electron density u_a satisfies

$$\inf_{x \in \mathbb{R}^3} u_a(x) \geq c_{a_c, M, \omega} > 0,$$

and by Remark 3 following Proposition 4.2

$$\|u_a - u_{a, R_n}\|_{L^\infty(B_1(0))} \leq C' e^{-\gamma(R_n - 1)}.$$

It follows that (6.2) holds for $R_n \geq R_0' := 1 + \gamma^{-1} \log(2C' c_{a_c, M, \omega}^{-1})$ and any $x \in B_1(0)$

$$u_{a, R_n}(x) \geq u_a(x) - C' e^{-\gamma(R_n - 1)} \geq c_{a_c, M, \omega} - \frac{c_{a_c, M, \omega}}{2} \geq \frac{c_{a_c, M, \omega}}{2} > 0.$$

The estimate (6.3) is shown by contradiction, so suppose that for all $R_0 > 0$

$$\inf_{a_c < a \leq a_0} \inf_{R_n \geq R_0} \inf_{m \in \mathcal{M}_{L^2}(M, \omega)} \inf_{x \in B_1(0)} u_{a, R_n, m}(x) = 0, \tag{6.4}$$

where $u_{a, R_n, m}$ solves (2.3a) corresponding to $m_{R_n} = m \cdot \chi_{B_{R_n}(0)}$.

Hence for each $k \in \mathbb{N}$ there exist sequences $(a_k) \subset (a_c, a_0]$, $R_{n_k} \uparrow \infty$, $\widetilde{m}_k \in \mathcal{M}_{L^2}(M, \omega)$ and $x_k \in B_1(0)$ such that $m_{k, R_{n_k}} = \widetilde{m}_k \cdot \chi_{B_{R_{n_k}}(0)}$ satisfies for all $k \in \mathbb{N}$

$$u_{a_k, R_{n_k}, \widetilde{m}_k}(x_k) \leq \frac{1}{k}.$$

For convenience, in this argument $u_{a_k, R_{n_k}, \widetilde{m}_k}$ and $m_{k, R_{n_k}}$ are referred to as u_k and m_k, respectively. By the Harnack inequality, for fixed $k \in \mathbb{N}$ and any $R' \geq 1$ there exists $C(R', a_0, M) > 0$ such that

$$\sup_{x \in B_{R'}(0)} u_k(x) \leq C \inf_{x \in B_{R'}(0)} u_k(x) \leq \frac{C(R', a_0, M)}{k}, \tag{6.5}$$

so it follows that u_k converges uniformly to 0 on any compact subset as $k \to \infty$. For $R > 0$ and $k \in \mathbb{N}$, define the energy functional acting on v satisfying $\nabla v \in L^2(B_R(0))$ and $v \in L^{10/3}(B_R(0))$ by

$$E(v; k, R) = \int_{B_R(0)} |\nabla v|^2 + \int_{B_R(0)} v^{10/3} - \int_{B_R(0)} (m_k * Y_{a_k}) v^2$$
$$+ \frac{1}{2} \int_{B_R(0)} \left(v^2 \cdot \chi_{B_R(0)} * Y_{a_k} \right) v^2 + \int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)^c} * Y_{a_k} \right) v^2. \tag{6.6}$$

Then consider the corresponding variational problem

$$I(k, R) = \inf \left\{ E(v; k, R) \,\middle|\, \nabla v \in L^2(B_R(0)), v \in L^{10/3}(B_R(0)), v|_{\partial B_R(0)} = u_k \right\}. \tag{6.7}$$

The construction of the energy and the boundary condition of (6.7) ensures that u_k is the unique minimiser of (6.7) for each $R > 0$. To prove this, observe that $E(v; k, R)$ can be expressed as

$$E(v; k, R) = \int_{B_R(0)} |\nabla v|^2 + \int_{B_R(0)} v^{10/3} + \int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)^c} * Y_{a_k} \right) v^2$$
$$+ \frac{1}{2} D_{a_k} \left(m_k - v^2 \chi_{B_R(0)}, m_k - v^2 \chi_{B_R(0)} \right) - \frac{1}{2} D_{a_k} (m_k, m_k).$$

As Y_{a_k} and the Yukawa interaction term are non-negative, it follows that

$$E(v; k, R) \geq \int_{B_R(0)} |\nabla v|^2 + \int_{B_R(0)} v^{10/3} - \frac{1}{2} D_{a_k}(m_k, m_k) \geq -\frac{1}{2} D_{a_k}(m_k, m_k) > -\infty,$$

so as $E(v; k, R)$ is bounded below, $I(k, R)$ is well-defined. Any minimising sequence v_n satisfies

$$\|\nabla v_n\|_{L^2(B_R(0))}^2 + \|v_n\|_{L^{10/3}(B_R(0))}^{10/3} \leq C(k, R, a_0, M),$$

hence there exists $v_{k,R}$ such that $\nabla v_{k,R} \in L^2(\mathbb{R}^3), v_{k,R} \in L^{10/3}(\mathbb{R}^3)$. Moreover, along a subsequence ∇v_n converges to $\nabla v_{k,R}$ weakly in $L^2(\mathbb{R}^3)$, v_n converges to $v_{k,R}$, weakly in $L^6(\mathbb{R}^3)$ and $L^{10/3}(\mathbb{R}^3)$, strongly in $L^p(B_R(0))$ for all $p \in [1, 6)$ and $R > 0$ and pointwise almost everywhere. Moreover, $v_{k,R}$ satisfies

$$E(v_{k,R}; k, R) = I(k, R),$$

and solves

$$-\Delta v_{k,R} + \frac{5}{3}v_{k,R}^{7/3} + \left(m_k - v_{k,R}^2 \cdot \chi_{B_R(0)} - u_k^2 \cdot \chi_{B_R(0)^c}\right) v_{k,R} = 0, \tag{6.8}$$

$$v_{k,R} = u_k \quad \text{on } \partial B_R(0).$$

It is straightforward to verify that u_k solves (6.8). Define the alternate minimisation problem

$$\inf\left\{ E(\sqrt{\rho}; k, R) \,\middle|\, \nabla\sqrt{\rho} \in L^2(\mathbb{R}^3), \rho \in L^{5/3}(\mathbb{R}^3), \rho \geq 0 \right\}. \tag{6.9}$$

Due to the strict convexity of $\rho \mapsto E(\sqrt{\rho}; k, R)$, it follows that $\rho_k = u_k^2$ is the unique minimiser of (6.9), hence u_k is the unique minimiser of (5.7).

As $u_k \to 0$ uniformly as $k \to \infty$, it follows that for any fixed $R > 0$

$$E(u_k; k, R) \to 0 \quad \text{as} \quad k \to \infty. \tag{6.10}$$

To verify (6.10), observe that

$$E(u_k; k, R) = \int_{B_R(0)} |\nabla u_k|^2 + \int_{B_R(0)} u_k^{10/3} - \int_{B_R(0)} (m_k * Y_{a_k}) u_k^2$$

$$+ \frac{1}{2} \int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)} * Y_{a_k}\right) u_k^2 + \int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)^c} * Y_{a_k}\right) u_k^2.$$

Clearly

$$0 \leq \int_{B_R(0)} u_k^{10/3} \leq CR^3 \|u_k\|_{L^\infty(B_R(0))}^{10/3} \to 0 \text{ as } k \to \infty. \tag{6.11}$$

The term $m_k * Y_{a_k}$ can be estimated by

$$\|m_k * Y_{a_k}\|_{L^\infty(\mathbb{R}^3)} \leq C(a_c, M), \tag{6.12}$$

where the constant $C(a_c, M)$ is independent of $k \in \mathbb{N}$. From (6.12) it follows that

$$\left| \int_{B_R(0)} (m_{k,j} * Y_{a_k}) u_k^2 \right| \leq \|m_k * Y_{a_k}\|_{L^\infty(\mathbb{R}^3)} \int_{B_R(0)} u_k^2$$

$$\leq Ca_c^{-3}MR^3 \|u_k\|_{L^\infty(B_R(0))}^2 \to 0 \text{ as } k \to \infty. \tag{6.13}$$

To show (6.12), let $\Gamma \subset \mathbb{R}^3$ be a semi-open unit cube centred at the origin, so $\mathbb{R}^3 = \{\Gamma + i \mid i \in \mathbb{Z}^3\}$. For any $x \in \mathbb{R}^3$

$$|(m_k * Y_{a_k})(x)| \leq \int_{\mathbb{R}^3} |m_k(x - y)| \frac{e^{-a_k|y|}}{|y|} \, \mathrm{d}y = \sum_{i \in \mathbb{Z}^3} \int_{\Gamma+i} |m_k(x - y)| \frac{e^{-a_k|y|}}{|y|} \, \mathrm{d}y$$

$$\leq C \sum_{i \in \mathbb{Z}^3} \|m_k\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \left\|\frac{e^{-a_k|\cdot|}}{|\cdot|}\right\|_{L^2(\Gamma+i)} \leq CM \sum_{i \in \mathbb{Z}^3} \left\|\frac{e^{-a_k|\cdot|}}{|\cdot|}\right\|_{L^2(\Gamma+i)}$$

$$\leq CM \sum_{i \in \mathbb{Z}^3} e^{-a_k|i|} \leq \frac{CM}{a_k^3} \leq \frac{CM}{a_c^3}. \tag{6.14}$$

As the estimate (6.14) is independent of $k \in \mathbb{N}$ and $x \in \mathbb{R}^3$, (6.12) holds. Estimating the remaining terms gives

$$\frac{1}{2} \int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)} * Y_{a_k}\right) u_k^2 \leq \|u_k\|_{L^\infty(B_R(0))}^4 D_{a_k}(\chi_{B_R(0)}, \chi_{B_R(0)}) \tag{6.15}$$

$$\leq Ca_c^{-2}R^3 \|u_k\|_{L^\infty(B_R(0))}^4 \to 0 \text{ as } k \to \infty, \tag{6.16}$$

$$\int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)^c} * Y_{a_k} \right) u_k^2 \leq \left\| u_k^2 \cdot \chi_{B_R(0)^c} * Y_{a_k} \right\|_{L^\infty(\mathbb{R}^3)} \int_{B_R(0)} u_k^2$$

$$\leq C R^3 \|u_k\|_{L^\infty(\mathbb{R}^3)}^2 \|Y_{a_k}\|_{L^1(\mathbb{R}^3)} \|u_k\|_{L^\infty(B_R(0))}^2$$

$$\leq \frac{C(a_0, M) R^3}{a_c^2} \|u_k\|_{L^\infty(B_R(0))}^2 \to 0 \text{ as } k \to \infty. \qquad (6.17)$$

For the final term, integration by parts yields

$$\int_{B_R(0)} |\nabla u_k|^2 = -\int_{B_R(0)} u_k \Delta u_k + \int_{\partial B_R(0)} u_k \frac{\partial u_k}{\partial n}$$

$$\leq C \|u_k\|_{W^{2,\infty}(\mathbb{R}^3)} (R^3 + R^2) \|u_k\|_{L^\infty(\overline{B_R(0)})}$$

$$\leq C(a_0, M) R^3 \|u_k\|_{L^\infty(B_R(0))} \to 0 \text{ as } k \to \infty. \qquad (6.18)$$

Collecting (6.11)–(6.18), it follows that for fixed $R > 0$, $E(u_k; k, R) \to 0$ as $k \to \infty$. A family of test functions $\varphi_{\varepsilon,k} \in H^1(B_R(0))$ is now constructed, satisfying the boundary condition $\varphi_{\varepsilon,k}|_{\partial B_R(0)} = u_k$ of (6.7) such that for sufficiently large $R > 0$ and small $\varepsilon > 0$, there exists a constant $C_1 > 0$ such that for all large $k \in \mathbb{N}$

$$E(\varphi_{\varepsilon,k}; k, R) \leq -C_1 < 0, \qquad (6.19)$$

contradicting the fact that $E(u_k; k, R) \to 0$ as $k \to \infty$, as (6.19) implies

$$E(u_k; k, R) \leq E(\varphi_{\varepsilon,k}; k, R) \leq -C_1 < 0.$$

Lemma 5.1 will be used to prove (6.19) by showing that there exists $R_0' \geq R_0$ and $k_1 \in \mathbb{N}$ such that choosing $R_n = R_0'$ and $k \geq k_1$ ensures

$$\int_{B_{4R_0'}(0)} |\nabla \psi_{R_0'}|^2 + \int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{4R_0'}(0)^c} - m_k \right) * Y_{a_k} \right) \psi_{R_0'}^2 \leq -1. \qquad (6.20)$$

Recall Lemma 5.1, that there exists $C_0 = C_0(a_c, a_0, \omega) > 0$ and $R_0 = R_0(a_c, a_0, \omega) > 0$ such that for any $a_c < a \leq a_0$ and $R_n \geq R_0$

$$\int_{\mathbb{R}^3} |\nabla \psi_{R_n}|^2 - D_a(m_{R_n}, \psi_{R_n}^2) \leq -C_0 R_n^3, \qquad (6.21)$$

The following term can be estimated and decomposed as

$$\int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{4R_n}(0)^c} \right) * Y_{a_k} \right) \psi_{R_n}^2 \leq \int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{4R_n}(0)^c} \right) * Y_{a_k} \right)$$

$$= \int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_n}(0)^c} \right) * Y_{a_k} \right) + \int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_n}(0) \setminus B_{4R_n}(0)} \right) * Y_{a_k} \right). \qquad (6.22)$$

The first term of (6.22) can be expressed as

$$\int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_n}(0)^c} \right) * Y_{a_k} \right) = \int_{B_{8R_n}(0)^c} u_k^2(y) \left(\int_{B_{4R_n}(0)} \frac{e^{-a_k|x-y|}}{|x-y|} \, dx \right) dy.$$

By the triangle inequality $|x - y| \geq \frac{|y|}{2}$, hence

$$\int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_n}(0)^c} \right) * Y_{a_k} \right)$$

$$\leq \|u_k\|^2_{L^\infty(\mathbb{R}^3)} \int_{B_{8R_n}(0)^c} \left(\int_{B_{4R_n}(0)} \frac{e^{-a_c|y|/2}}{|y|} \, dx \right) dy = C R_n^3 \int_{B_{8R_n}(0)^c} \frac{e^{-a_c|y|/2}}{|y|} \, dy$$

$$= C a_c^{-2} R_n^3 \left(1 + 4 a_c R_n \right) e^{-4 a_c R_n} \leq C a_c^{-2} R_n^3 e^{-2 a_c R_n}.$$

As $e^{-2a_c R_n} \to 0$ as $R_n \to \infty$, there exists $R_2 > 0$ such that for $R_n \geq R_2$

$$\int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_n}(0)^c} \right) * Y_{a_k} \right) \leq C a_c^{-2} R_n^3 e^{-2 a_c R_n} \leq \frac{C_0}{4} R_n^3. \tag{6.23}$$

Now define $R_0' = \max\{R_0, R_2, (2C_0)^{-1/3}\}$ and choose $R_n = R_0'$. The second term of (6.22) can be estimated using Young's inequality for convolutions

$$\int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_0'}(0) \setminus B_{4R_0'}(0)} \right) * Y_{a_k} \right) \leq \int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_0'}(0)} \right) * Y_{a_k} \right)$$

$$\leq C R_0'^3 \|Y_{a_k}\|_{L^1(\mathbb{R}^3)} \|u_k\|^2_{L^\infty(B_{8R_0'}(0))} \leq C a_c^{-2} R_0'^3 \|u_k\|^2_{L^\infty(B_{8R_0'}(0))}.$$

As $u_k \to 0$ on compact sets, there exists $k_1 \in \mathbb{N}$ such that $k \geq k_1$ ensures that

$$\int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_0'}(0) \setminus B_{4R_0'}(0)} \right) * Y_{a_k} \right) \leq C a_c^{-2} R_0'^3 \|u_k\|^2_{L^\infty(B_{8R_0'}(0))} \leq \frac{C_0}{4} R_0'^3. \tag{6.24}$$

Choose $R_n = R_0'$ and recall that $R_{n_k} \uparrow \infty$, hence there exists $k_2 \in \mathbb{N}$ such that $R_{n_k} \geq R_0'$ for all $k \geq k_2$, so it follows that $m_k \geq m_{R_n}$. Collecting the estimates (6.21), (6.22)–(6.24) with $R_n = R_0'$ and observing that $\frac{C_0}{4} R_0'^3 \geq 1$ yields the desired estimate (6.20)

$$\int_{B_{4R_0'}(0)} |\nabla \psi_{R_0'}|^2 + \int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{4R_0'}(0)^c} - m_k \right) * Y_{a_k} \right) \psi_{R_0'}^2$$

$$\leq \int_{\mathbb{R}^3} |\nabla \psi_{R_0'}|^2 - D_a\left(m_{R_0'}, \psi_{R_0'}^2\right) + \int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_0'}(0)^c} \right) * Y_{a_k} \right)$$

$$+ \int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_0'}(0) \setminus B_{4R_0'}(0)} \right) * Y_{a_k} \right)$$

$$\leq -C_0 R_0'^3 + \frac{C_0}{4} R_0'^3 + \frac{C_0}{4} R_0'^3 = -\frac{C_0}{2} R_0'^3 \leq -1.$$

Now choose $R = 4R_0' + 2$ such that $\psi = \psi_{R_0'} \in C_c^\infty(B_{R-2}(0))$ satisfies the estimate (6.20) for all $a_c < a \leq a_0$. Then let $\xi \in C^\infty(\mathbb{R}^3)$ satisfy $0 \leq \xi \leq 1$, $\xi = 1$ on $B_{R-1}^c(0)$, $\xi = 0$ on $B_{R-2}(0)$ and for $\varepsilon > 0$, define $\varphi_{\varepsilon,k} \in H^1(\mathbb{R}^3)$ by

$$\varphi_{\varepsilon,k}(x) = \varepsilon \psi(x) + \xi(x) u_k(x). \tag{6.25}$$

It follows from the definition that $\varphi_{\varepsilon,k}$ satisfies the boundary condition from (6.7), that $\varphi_{\varepsilon,k}|_{\partial B_R(0)} = u_k$. Observe that as ψ and $\xi \cdot u_k$ have disjoint support, the energy $E(\varphi_{\varepsilon,k}; k, R)$ can be decomposed as

$$E(\varphi_{\varepsilon,k}; k, R) = E(\varepsilon \psi; k, R) + E(\xi u_k; k, R)$$

$$+ \varepsilon^2 \int_{B_R(0)} \left((\xi u_k)^2 \cdot \chi_{B_R(0)} * Y_{a_k} \right) \psi^2.$$

Recall that ψ satisfies (6.20), so for $0 < \varepsilon \leq 1$

$$E(\varepsilon\psi; k, R) + \varepsilon^4 = \varepsilon^2 \left(\int_{B_R(0)} |\nabla \psi|^2 + \int_{B_R(0)} \left((u_k^2 \cdot \chi_{B_R(0)^c} - m_k) * Y_{a_k} \right) \psi^2 \right)$$

$$+ \varepsilon^{10/3} \int_{B_R(0)} \psi^{10/3} + \frac{\varepsilon^4}{2} \int_{B_R(0)} \left(\psi^2 \cdot \chi_{B_R(0)} * Y_{a_k} \right) \psi^2 + \varepsilon^4$$

$$\leq -\varepsilon^2 + C\varepsilon^{10/3} R^3 + C\varepsilon^4 a_k^{-2} R^3 + \varepsilon^4$$

$$\leq -\varepsilon^2 + C\varepsilon^4 =: -\varepsilon^2 + C_3 \varepsilon^4.$$

Choosing $\varepsilon = \varepsilon_0 = \min\{1, (2C_3)^{-1/2}\}$ implies that (6.26) holds

$$E(\varepsilon_0 \psi; k, R) + \varepsilon_0^4 \leq -\varepsilon_0^2 + C_3 \varepsilon_0^4 \leq -\frac{\varepsilon_0^2}{2} =: -C_1 < 0. \tag{6.26}$$

Now consider

$$E(\xi u_k; k, R) = \int_{B_R(0)} |\nabla(\xi u_k)|^2 + \int_{B_R(0)} (\xi u_k)^{10/3} - \int_{B_R(0)} (m_k * Y_{a_k})(\xi u_k)^2$$

$$+ \frac{1}{2} \int_{B_R(0)} \left((\xi u_k)^2 \cdot \chi_{B_R(0)} * Y_{a_k} \right) (\xi u_k)^2 + \int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)^c} * Y_{a_k} \right) (\xi u_k)^2.$$

Using that $0 \leq \xi \leq 1$, $|\nabla \xi| \in L^\infty(\mathbb{R}^3)$, $u_k \to 0$ as $k \to \infty$ and following the proof of (6.10), it follows that $E(\xi u_k; k, R) \to 0$ as $k \to \infty$. For the remaining term

$$0 \leq \varepsilon_0^2 \int_{B_R(0)} \left((\xi u_k)^2 \cdot \chi_{B_R(0)} * Y_{a_k} \right) \psi^2 \leq C\varepsilon_0^2 \|u_k\|_{L^\infty(B_R(0))}^2 \|Y_{a_k}\|_{L^1(\mathbb{R}^3)} \int_{B_R(0)} \psi^2$$

$$= \frac{C\varepsilon_0^2}{a_c^2} \|u_k\|_{L^\infty(B_R(0))}^2 \to 0 \text{ as } k \to \infty. \tag{6.27}$$

It follows that there exists $k_2 \in \mathbb{N}$ such that for all $k \geq k_2$

$$E(\xi u_k; k, R) + \varepsilon_0^2 \int_{B_R(0)} \left((\xi u_k)^2 \cdot \chi_{B_R(0)} * Y_{a_k} \right) \psi^2 \leq \varepsilon_0^4. \tag{6.28}$$

Combining (6.26) and (6.28), for $k \geq \max\{k_1, k_2\}$ yields the desired estimate (6.19).

$$E(\varphi_{\varepsilon_0, k}; k, R) = E(\varepsilon_0 \psi; k, R) + E(\xi u_k; k, R)$$

$$+ \varepsilon_0^2 \int_{B_R(0)} \left((\xi u_k)^2 \cdot \chi_{B_R(0)} * Y_{a_k} \right) \psi^2$$

$$\leq E(\varepsilon_0 \psi; k, R) + \varepsilon_0^4 \leq -C_1 < 0,$$

which contradicts the initial assumption (6.4). $\qquad \square$

Proof of Proposition 5.5. The estimate (5.56) is shown by contradiction, so suppose there exists $a_0 > a_c$ such that

$$\inf_{a_c < a \leq a_0} \inf_{m \in \mathcal{M}_{L^2}(M, \omega)} \inf_{x \in \mathbb{R}^3} u_{a,m}(x) = 0, \tag{6.29}$$

hence for each $k \in \mathbb{N}$, there exists $a_k \in (a_c, a_0]$, $m_k \in \mathcal{M}_{L^2}(M, \omega)$ and $x_k \in \mathbb{R}^3$ such that $u_{a_k, m_k}(x_k) \leq \frac{1}{k}$. Without loss of generality, assume that $x_k = 0$ for all $k \in \mathbb{N}$, otherwise translate u_{a_k, m_k}. For convenience, u_{a_k, m_k} will be referred to as u_k in this argument. By the Harnack inequality, it follows that u_k converges uniformly to 0 on compact sets.

For $R > 0$ and $k \in \mathbb{N}$, define the energy functional acting on v satisfying $\nabla v \in L^2(B_R(0))$ and $v \in L^{10/3}(B_R(0))$ by

$$E(v; k, R) = \int_{B_R(0)} |\nabla v|^2 + \int_{B_R(0)} v^{10/3} - \int_{B_R(0)} (m_k * Y_{a_k}) v^2$$
$$+ \frac{1}{2} \int_{B_R(0)} \left(v^2 \cdot \chi_{B_R(0)} * Y_{a_k} \right) v^2 + \int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)^c} * Y_{a_k} \right) v^2. \quad (6.30)$$

Then consider the corresponding variational problem

$$I(k, R) = \inf \left\{ E(v; k, R) \,\middle|\, \nabla v \in L^2(B_R(0)), v \in L^{10/3}(B_R(0)), v|_{\partial B_R(0)} = u_k \right\}. \quad (6.31)$$

The construction of the energy (6.30) and the boundary condition of (6.31) ensures that u_k is the unique minimiser of (6.31) for each $R > 0$. It follows that for any fixed $R > 0$, $I(k, R) \to 0$ as $k \to \infty$. Then by following the construction used in the proof of Lemma 6.1, there exists $R > 0$ and $\varphi_{\varepsilon,k}$ such that for sufficiently small $\varepsilon > 0$ and sufficiently large $k \in \mathbb{N}$

$$I(k, R) = E(u_k; k, R) \leq E(\varphi_{\varepsilon,k}; k, R) \leq -C_1 < 0,$$

which contradicts the fact that $I(k, R) \to 0$ as $k \to \infty$, hence the desired estimate (5.56) holds.

Consequently, as for all $a > 0$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, the electron density satisfies $\inf u_a > 0$, the argument presented in [6, Chapter 6] can be applied verbatim to guarantee the uniqueness of the corresponding ground state (u_a, ϕ_a). $\qquad \square$

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