

Original citation:

Nazar, Faizan Q. and Ortner, Christoph. (2016) Locality of the Thomas-Fermi-von Weizsäcker Equations. Archive for Rational Mechanics and Analysis, 224 (3). 817.

Permanent WRAP URL:

<http://wrap.warwick.ac.uk/84814>

Copyright and reuse:

The Warwick Research Archive Portal (WRAP) makes this work of researchers of the University of Warwick available open access under the following conditions.

This article is made available under the Creative Commons Attribution 4.0 International license (CC BY 4.0) and may be reused according to the conditions of the license. For more details see: <http://creativecommons.org/licenses/by/4.0/>

A note on versions:

The version presented in WRAP is the published version, or, version of record, and may be cited as it appears here.

For more information, please contact the WRAP Team at: wrap@warwick.ac.uk



Locality of the Thomas–Fermi–von Weizsäcker Equations

F. Q. NAZAR & C. ORTNER

Communicated by G. FRIESECKE

Abstract

We establish a pointwise stability estimate for the Thomas–Fermi–von Weizsäcker (TFW) model, which demonstrates that a local perturbation of a nuclear arrangement results also in a local response in the electron density and electrostatic potential. The proof adapts the arguments for existence and uniqueness of solutions to the TFW equations in the thermodynamic limit by Catto et al. (The mathematical theory of thermodynamic limits: Thomas–Fermi type models. Oxford mathematical monographs. The Clarendon Press, Oxford University Press, New York, 1998). To demonstrate the utility of this combined locality and stability result we derive several consequences, including an exponential convergence rate for the thermodynamic limit, partition of total energy into exponentially localised site energies (and consequently, exponential locality of forces), and generalised and strengthened results on the charge neutrality of local defects.

1. Introduction

Locality properties of electronic structure models are a key premise in certain state of the art numerical algorithms. A well-established example is “near-sightedness”, a locality property of the density matrix which gives rise to linear scaling algorithms for Kohn–Sham type models [6, 24, 25, 38]. A stronger notion is the locality of the mechanical response, which is a fundamental premise underpinning the construction of interatomic potentials and of multi-scale algorithms such as hybrid QM/MM schemes [17] (here, it is termed “strong locality”). This latter category of locality is less well studied, the only result in this direction being the locality of non-selfconsistent tight binding models [14].

The aim of the present work is to establish the locality properties satisfied by the Thomas–Fermi–von Weizsäcker (TFW) model. Our main technical result to achieve this is the following pointwise stability estimate for the TFW equations,

which establishes the locality of the electron response to changes in the nuclear configuration. Compared with [14] it is noteworthy that our result takes Coulomb interaction fully into account. Rigorous statements, under different conditions, are given in Theorems 3.1 and 3.2.

Theorem. For $i = 1, 2$ let $m_i \in L^\infty(\mathbb{R}^3)$ represent nuclear charge distributions satisfying

$$m_i \geq 0 \quad \text{and} \quad \lim_{R \rightarrow \infty} \frac{1}{R} \inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m_i(z) \, dz = +\infty.$$

Let the corresponding ground state electron densities and electrostatic potentials, denoted by $u_i, \phi_i : \mathbb{R}^3 \rightarrow \mathbb{R}$, satisfy the TFW equations,

$$\begin{aligned} -\Delta u_i + \frac{5}{3} u_i^{7/3} - \phi_i u_i &= 0, \\ -\Delta \phi_i &= 4\pi (m_i - u_i^2). \end{aligned}$$

Then there exists $C, \gamma > 0$ such that for all $y \in \mathbb{R}^3$

$$|(u_1 - u_2)(y)| + |(\phi_1 - \phi_2)(y)| \leq C \left(\int_{\mathbb{R}^3} |(m_1 - m_2)(x)|^2 e^{-2\gamma|x-y|} \, dx \right)^{1/2}. \quad (1.1)$$

In the remainder of the article we explore some of the consequences of this locality result: In Proposition 4.1 we obtain new estimates on finite-domain approximations which yield exponential decay of surface energies as well as an exponential convergence rate for the thermodynamic limit. In Corollary 4.1 we show that (1.1) gives rise to rigorous results that match, and substantially generalise, the Thomas–Fermi theory of impurity screening in metals [2, 28]. In Theorem 4.1 we strengthen existing results on the neutrality of the TFW model [10]. In all these results, general (condensed) nuclear arrangements are treated.

A striking application of (1.1) is that it allows us to decompose energy into local contributions from which we obtain local site energy potentials: Given a countable collection of nuclei $Y = (Y_j)_{j \in \mathbb{N}} \subset \mathbb{R}^3$ we construct an energy density $\mathcal{E}(Y; x)$ which allows us to define the TFW energy $\int_{\Omega} \mathcal{E}(Y; x) \, dx$ of an arbitrary volume $\Omega \subset \mathbb{R}^3$ in a meaningful way. This then motivates us to define site energies

$$E_j(Y) := \int_{\mathbb{R}^3} \varphi_j(x) \mathcal{E}(Y; x) \, dx,$$

where $(\varphi_j)_{j \in \mathbb{N}}$ is a smooth partition of unity of \mathbb{R}^3 , which can be constructed in such a way that E_j are permutation and isometry invariant and most crucially, E_j are *local* in the sense that

$$\left| \frac{\partial E_j(Y)}{\partial Y_k} \right| \leq C e^{-\gamma|Y_j - Y_k|}, \quad (1.2)$$

for some $C, \gamma > 0$. The rigorous statement of this result is given in Theorem 4.2. An analogous result has recently been proven for a tight binding model in [14].

This result not only gives a strong justification for the construction of classical short-ranged interatomic potentials in metals, but in fact it allows us to treat the TFW mechanical response as if it emanated from such a classical potential. For example, (i) the analysis of the Cauchy–Born continuum limit [37, Page 5] applies directly to the TFW model; and (ii) we can generalise in [13] the analysis of variational problems for the mechanical response to defects in an infinite crystal [19].

The remainder of this article is organised as follows: In Section 2 we recall the definition of the TFW model and summarise the relevant existing results. In Section 3 we state the main technical results, including the rigorous statement of the stability result (1.1). In Section 4 we present applications. Concluding remarks are made in Section 5, followed by the detailed proofs of the results in Section 6.

Remark 1. We conclude the introduction with a remark about the analytical context of this work. The TFW equations for the electron density and potential is a coupled Schrödinger–Poisson system. Other systems of this class can be found in semiconductor physics [34, 43, 45]. We also note that Thomas–Combes estimates give conditions under which eigenfunctions of a Schrödinger operator decay exponentially [1, 16]. While the results obtained for these systems are similar, the corresponding equations have different structure, hence the analytical techniques used to study them differ considerably.

The closest existing result to (1.1) we have found is [8, Theorem 4.6], which shows the exponential decay of the electron density away from the boundary of a crystal. Both (1.1) and [8, Theorem 4.6] utilise the uniqueness of the TFW equations to prove stability estimates. In Section 4.1, we use Proposition 4.1 to generalise [8, Theorem 4.6]. \square

2. The TFW Model

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

$$L_{\text{loc}}^p(\mathbb{R}^3) := \left\{ f : \mathbb{R}^3 \rightarrow \mathbb{R} \mid \forall K \subset \mathbb{R}^3 \text{ compact, } f \in L^p(K) \right\} \quad \text{and}$$

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

For $k \in \mathbb{N}$, $H_{\text{loc}}^k(\mathbb{R}^3)$, $H_{\text{unif}}^k(\mathbb{R}^3)$ are defined analogously. For a multi-index $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, we 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

$$D(f, g) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{f(x)g(y)}{|x-y|} \, dx \, dy = \int_{\mathbb{R}^3} \left(f * \frac{1}{|\cdot|} \right) (y) g(y) \, dy. \quad (2.1)$$

This is finite due to the Hardy–Littlewood–Sobolev estimate [3]

$$|D(f, g)| \leq C \|f\|_{L^{6/5}(\mathbb{R}^3)} \|g\|_{L^{6/5}(\mathbb{R}^3)}. \quad (2.2)$$

Let $m \in L^{6/5}(\mathbb{R}^3)$, $m \geq 0$ denote the charge density of a finite nuclear cluster, then the corresponding TFW energy functional is defined, for $v \in H^1(\mathbb{R}^3)$, by

$$E^{\text{TFW}}(v, m) = C_W \int_{\mathbb{R}^3} |\nabla v|^2 + C_{\text{TF}} \int_{\mathbb{R}^3} v^{10/3} + \frac{1}{2} D(m - v^2, m - v^2). \quad (2.3)$$

The function v corresponds to the positive square root of the electron density. The first two terms of $E^{\text{TFW}}(v, m)$ model the kinetic energy of the electrons while the third term models the Coulomb energy. We remark that this definition of the Coulomb energy is only valid for smeared nuclei. We can rescale the energy to ensure $C_W = C_{\text{TF}} = 1$.

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

$$\begin{aligned} \text{(H1)} \quad & \sup_{x \in \mathbb{R}^3} \int_{B_1(x)} m(z) \, dz < \infty, \\ \text{(H2)} \quad & \lim_{R \rightarrow \infty} \inf_{x \in \mathbb{R}^3} \frac{1}{R} \int_{B_R(x)} m(z) \, dz = \infty. \end{aligned}$$

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.

Let $R_n \uparrow \infty$ and define the truncated nuclear distribution $m_{R_n} = m \cdot \chi_{B_{R_n}(0)}$, then the minimisation problem

$$I^{\text{TFW}}(m_{R_n}) = \inf \left\{ E^{\text{TFW}}(v, m_{R_n}) \mid v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_{R_n} \right\}$$

possesses a unique minimiser u_{R_n} . The charge constraint ensures that the system is neutral. Further, u_{R_n} solves the corresponding Euler–Lagrange equation, which can be expressed as the coupled system

$$-\Delta u_{R_n} + \frac{5}{3} u_{R_n}^{7/3} - \phi_{R_n} u_{R_n} = 0, \quad (2.4a)$$

$$-\Delta \phi_{R_n} = 4\pi (m_{R_n} - u_{R_n}^2). \quad (2.4b)$$

By the proof of [12, Corollary 2.7, Theorem 6.10], it follows that

$$\|u_{R_n}\|_{H^1_{\text{unif}}(\mathbb{R}^3)} + \|\phi_{R_n}\|_{L^2_{\text{unif}}(\mathbb{R}^3)} \leq C, \quad (2.5)$$

where C is independent of R_n . Consequently, (2.5) implies that along a subsequence (u_{R_n}, ϕ_{R_n}) converge to (u, ϕ) . Passing to the limit in (2.4) yields the following result.

Theorem 2.1. [12, Theorem 6.10] *Let $m \in L^1_{\text{unif}}(\mathbb{R}^3)$, $m \geq 0$ satisfy (H1)–(H2), then there exists a unique solution $(u, \phi) \in L^\infty(\mathbb{R}^3) \times L^1_{\text{unif}}(\mathbb{R}^3)$, up to the sign of u , of*

$$-\Delta u + \frac{5}{3}u^{7/3} - \phi u = 0, \quad (2.6a)$$

$$-\Delta \phi = 4\pi (m - u^2), \quad (2.6b)$$

in the distributional sense. In addition, $\inf u > 0$.

Definition 1. For any nuclear configuration m satisfying (H1)–(H2), we refer to (u, ϕ) solving (2.6) as the ground state corresponding to m . \square

Remark 2. A concise proof of uniqueness of the TFW equations is given in [7] under the assumption that m is smooth and hence $u, \phi \in W^{1,\infty}(\mathbb{R}^3)$, which simplifies the earlier proof given in [12]. \square

In the next section, we discuss results that can be obtained by generalising the proof of Theorem 2.1.

3. Main Results

3.1. Uniform Regularity Estimates

In the proof of our main results in the next section we employ regularity estimates that refine those of [12], and may be of independent interest.

Other than Proposition 3.1, our estimates rely on uniform variants of (H1)–(H2) and it turns out that (H2) may then be simplified without loss of generality; see Lemma 6.1 for more details. Given $M, \omega_0, \omega_1 > 0$, let $\omega = (\omega_0, \omega_1)$ and define the class of nuclear configurations

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

As each nuclear distribution $m \in \mathcal{M}_{L^2}(M, \omega)$ satisfies (H1)–(H2), Theorem 2.1 guarantees the existence of corresponding ground states (u, ϕ) . We adapt the proof of existence of Theorem 2.1 to show that 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. *For any nuclear distribution $m : \mathbb{R}^3 \rightarrow \mathbb{R}_{\geq 0}$, satisfying*

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

there exists (u, ϕ) solving (2.6) and satisfying $u \geq 0$ and

$$\|u\|_{H_{\text{unif}}^4(\mathbb{R}^3)} \leq C \left(1 + M^{15/4}\right), \quad (3.2)$$

$$\|\phi\|_{H_{\text{unif}}^2(\mathbb{R}^3)} \leq C \left(1 + M^{3/2}\right). \quad (3.3)$$

Proposition 3.2. *There exists $c_{M,\omega} > 0$ such that for all $m \in \mathcal{M}_{L^2}(M, \omega)$ the corresponding ground state (u, ϕ) is unique and the electron density u satisfies*

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

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

$$\mathcal{M}_{H^k}(M, \omega) = \left\{ m \in H_{\text{unif}}^k(\mathbb{R}^3) \mid \|m\|_{H_{\text{unif}}^k(\mathbb{R}^3)} \leq M, \right. \\ \left. \forall R > 0 \inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m(z) \, dz \geq \omega_0 R^3 - \omega_1 \right\}.$$

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

Corollary 3.1. *Suppose $k \in \mathbb{N}_0$ and $m \in \mathcal{M}_{H^k}(M, \omega)$, then the corresponding solution (u, ϕ) to (2.6) satisfies*

$$\|u\|_{H_{\text{unif}}^{k+4}(\mathbb{R}^3)} + \|\phi\|_{H_{\text{unif}}^{k+2}(\mathbb{R}^3)} \leq C(k, M, \omega). \quad (3.5)$$

3.2. Pointwise Stability and Locality

We now discuss our main result, a pointwise stability estimate for (2.6) which reveals a generic locality of the TFW interaction. To establish this result, we adapt the proof of uniqueness of the TFW equations in [7, 12], specialising the class of test functions to

$$H_\gamma = \left\{ \xi \in H^1(\mathbb{R}^3) \mid |\nabla \xi(x)| \leq \gamma |\xi(x)| \, \forall x \in \mathbb{R}^3 \right\} \quad (3.6)$$

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

Theorem 3.1. *Let $m_1 \in \mathcal{M}_{L^2}(M, \omega)$, and let (u_1, ϕ_1) . Also, let $m_2 : \mathbb{R}^3 \rightarrow \mathbb{R}_{\geq 0}$ satisfy $\|m_2\|_{L_{\text{unif}}^2(\mathbb{R}^3)} \leq M'$ and suppose there exists (u_2, ϕ_2) solving (2.6) corresponding to m_2 , satisfying $u_2 \geq 0$ and*

$$\|u_2\|_{H_{\text{unif}}^4(\mathbb{R}^3)} + \|\phi_2\|_{H_{\text{unif}}^2(\mathbb{R}^3)} \leq C(M'). \quad (3.7)$$

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

$$\int_{\mathbb{R}^3} \left(\sum_{|\alpha_1| \leq 4} |\partial^{\alpha_1}(u_1 - u_2)|^2 + \sum_{|\alpha_2| \leq 2} |\partial^{\alpha_2}(\phi_1 - \phi_2)|^2 \right) \xi^2 \leq C \int_{\mathbb{R}^3} (m_1 - m_2)^2 \xi^2. \quad (3.8)$$

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

$$\sum_{|\alpha| \leq 2} |\partial^\alpha(u_1 - u_2)(y)|^2 + |(\phi_1 - \phi_2)(y)|^2 \leq C \int_{\mathbb{R}^3} |(m_1 - m_2)(x)|^2 e^{-2\gamma|x-y|} dx. \quad (3.9)$$

Remark 3. Since we do not assume that $m_2 \in \mathcal{M}_{L^2}(M', \omega')$, we can not guarantee the uniqueness of the corresponding solution (u_2, ϕ_2) . \square

We can generalise Theorem 3.1 to obtain higher-order pointwise estimates, but this requires *both* $\inf u_1, \inf u_2 > 0$, hence we need to assume $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$ for some $k \in \mathbb{N}_0$.

Theorem 3.2. Let $k \in \mathbb{N}_0$ and $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$. Consider the corresponding ground states (u_1, ϕ_1) , (u_2, ϕ_2) and define

$$w = u_1 - u_2, \quad \psi = \phi_1 - \phi_2, \quad R_m = 4\pi(m_1 - m_2).$$

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

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

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

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(y)|^2 \leq C \int_{\mathbb{R}^3} \sum_{|\beta| \leq k} |\partial^\beta R_m(x)|^2 e^{-2\gamma|x-y|} dx. \quad (3.11)$$

Remark 4. It is possible to generalise Theorem 3.1 to treat nuclei described by a non-negative measure m on \mathbb{R}^3 satisfying

$$\sup_{x \in \mathbb{R}^3} m(B_1(x)) \leq M, \quad (\text{H1}') \quad (3.12)$$

and there exist $\omega_0 > 0$, $\omega_1 \geq 0$ such that for all $R > 0$

$$\inf_{x \in \mathbb{R}^3} m(B_R(x)) \geq \omega_0 R^3 - \omega_1. \quad (\text{H2}') \quad (3.13)$$

The existence and uniqueness of a corresponding ground state (u, ϕ) is guaranteed by [12, Theorem 6.10]. We believe that the arguments used to show [12, Lemma 5.5] and Theorem 3.1 can be adapted to show pointwise estimates similar to (3.8)–(3.9) when m_1, m_2 satisfy (H1')–(H2') and that $m_1 - m_2$ is absolutely continuous with respect to the Lebesgue measure on \mathbb{R}^3 , with a density belonging to $L^2_{\text{unif}}(\mathbb{R}^3)$.

This result is not sufficient to consider the response of the ground state to a perturbation of point nuclei, though it may be possible to treat this using an approximation to the identity or by applying similar techniques. \square

4. Applications

4.1. Thermodynamic Limit Estimates

The following result provides an estimate for comparing the infinite ground state with its finite approximation, over compact sets, thus providing explicit rates of convergence for the thermodynamic limit. This is discussed in Remark 5.

Interpreted differently, the result yields estimates on the decay of the perturbation from the bulk electronic structure at a domain boundary, generalising the exponential decay estimate [8, Theorem 4.6] to arbitrary open $\Omega \subset \mathbb{R}^3$ and general $m \in \mathcal{M}_{L^2}(M, \omega)$.

Proposition 4.1. *Let $m \in \mathcal{M}_{L^2}(M, \omega)$ and (u, ϕ) be the corresponding ground state. Further, let $\Omega \subset \mathbb{R}^3$ be open and suppose there exists $m_\Omega : \mathbb{R}^3 \rightarrow \mathbb{R}_{\geq 0}$ such that $m_\Omega = m$ on Ω and $\|m_\Omega\|_{L^2_{\text{unif}}(\mathbb{R}^3)} \leq M$ (e.g., $m_\Omega = m\chi_\Omega$), then there exists (u_Ω, ϕ_Ω) solving (2.6) with $m = m_\Omega$, $u_\Omega \geq 0$ and $C = C(M, \omega)$, $\gamma = \gamma(M, \omega) > 0$, independent of Ω , such that for all $y \in \Omega$*

$$\sum_{|\alpha| \leq 2} |\partial^\alpha (u - u_\Omega)(y)| + |(\phi - \phi_\Omega)(y)| \leq Ce^{-\gamma \text{dist}(y, \partial\Omega)}. \quad (4.1)$$

Remark 5. Let $R > 0$ and $R_n \uparrow \infty$, then applying Proposition 4.1 with $\Omega = B_{R_n}(0)$ and $m_\Omega = m_{R_n}$ gives a rate of convergence for the finite approximation (u_{R_n}, ϕ_{R_n}) , solving (2.4), to the ground state (u, ϕ) ,

$$\|u - u_{R_n}\|_{W^{2,\infty}(B_R)(0)} + \|\phi - \phi_{R_n}\|_{L^\infty(B_R)(0)} \leq Ce^{-\gamma(R_n - R)}. \quad (4.2)$$

This strengthens the result that (u_{R_n}, ϕ_{R_n}) converges to (u, ϕ) pointwise almost everywhere along a subsequence [12]. \square

4.2. Locality of the Charge Response

The following result shows that the decay properties of the nuclear perturbation are inherited by the response of the ground state.

Corollary 4.1. *Let $k \in \mathbb{N}_0$ and $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$. Consider the corresponding ground states (u_1, ϕ_1) , (u_2, ϕ_2) and define*

$$w = u_1 - u_2, \quad \psi = \phi_1 - \phi_2, \quad R_m = 4\pi(m_1 - m_2).$$

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

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(x)| + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(x)| \leq C e^{-\gamma|x|}. \quad (4.3)$$

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 $C = C(r, k, M, \omega) > 0$ such that*

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(x)| + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(x)| \leq C(1 + |x|)^{-r}. \quad (4.4)$$

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

$$\|w\|_{H^{k+4}(\mathbb{R}^3)} + \|\psi\|_{H^{k+2}(\mathbb{R}^3)} \leq C \|R_m\|_{H^k(\mathbb{R}^3)}. \quad (4.5)$$

Remark 6. For some of our comparison results, we require only $m_1 \in \mathcal{M}_{L^2}(M, \omega)$ but impose weaker assumptions on m_2 . This would not generalise Corollary 4.1 since any of the decay assumptions in (1–3) already imply that $m_2 \in \mathcal{M}_{L^2}(M, \omega')$ for some ω' . \square

Remark 7. The estimate (4.3) can be used to study the full non-linear response of the ground state to a nuclear impurity. We compare this to the results from the Thomas–Fermi (TF) [2, 28, 39] and TFW [18, 29, 35, 40] theories of screening.

Consider a nuclear arrangement $m_1 \in \mathcal{M}_{L^2}(M, \omega)$ and model a nuclear impurity at the origin with positive charge Z by $Z\eta(x)$, where $\eta \in C_c^\infty(\mathbb{R}^3)$, $\eta \geq 0$ and $\int \eta = 1$. Then define the perturbed system by $m_2 = m_1 + Z\eta \in \mathcal{M}_{L^2}(M_1, \omega_1)$ and consider the corresponding TFW ground states (u_1, ϕ_1) and (u_2, ϕ_2) , respectively. From (4.3) of Corollary 4.1 it follows that

$$\sum_{|\alpha| \leq 2} |\partial^\alpha (u_1 - u_2)(x)| + |(\phi_1 - \phi_2)(x)| \leq CZ e^{-\gamma|x|}, \quad (4.6)$$

We now compare (4.6) with existing results from the TF and TFW theories of screening. These models consider the formal linear response (n, V) of the electron density and potential to a nuclear impurity at the origin, modelled by the Dirac distribution $Z\delta_0$, in a uniform electron gas. In both models, V satisfies the linear equation

$$-\Delta V = 4\pi [n + Z\delta_0],$$

while n solves either the linearised TF or TFW equations. In the TF model, V and n are shown to satisfy [28, Page 112], [2, Page 342]

$$V(x) = Z \frac{e^{-k_s|x|}}{|x|}, \quad n(x) = -\frac{Zk_s^2}{4\pi} \frac{e^{-k_s|x|}}{|x|}, \quad (4.7)$$

where $k_s > 0$ is a material-dependent constant called the inverse screening length. In the TFW model, V and n satisfy [18, 29, 35, 40]

$$\begin{aligned} V(x) &= \frac{Z}{4\alpha\beta|x|} e^{-\alpha|x|} \left((\alpha + \beta)^2 e^{\beta|x|} - (\alpha - \beta)^2 e^{-\beta|x|} \right), \\ n(x) &= -\frac{(\alpha^2 - \beta^2)^2 Z}{\alpha\beta|x|} e^{-\alpha|x|} \left(e^{\beta|x|} - e^{-\beta|x|} \right), \end{aligned} \quad (4.8)$$

where $\alpha \in \mathbb{R}$, $\beta \in \mathbb{C}$ satisfy $0 < |\beta| < \alpha$. The constants α, β depend on the material and the coefficient C_W , which appears in the definition of the TFW energy (2.3). There is a critical value of C_W below which $\beta > 0$ and above which β is complex, the latter case introduces oscillations in the potential and electron density. In either case, both the TF and TFW models exhibit screening due to the presence of the exponential term appearing in (4.7)–(4.8).

The lack of a factor of the form $\frac{1}{|x|}$ in (4.6) can be attributed to using a smeared nuclear description for the impurity as opposed to a point description in (4.7)–(4.8). Other than this, the similarity of (4.6) to (4.7) suggests that the constant γ in (4.6) may be interpreted as the inverse screening length. In this paper we show there exists $\gamma > 0$ satisfying (4.6), however we do not provide any estimates for its value.

The estimate (4.6) shows that screening occurs in the TFW model, without any approximations made to the model and without any restrictions on the nuclear configurations (other than (H1)–(H2)). It should be noted that although (4.6) agrees with existing results from the TF theory of screening, in metals often the effects of screening are weaker. For metals, instead of an exponentially decaying screening factor, Friedel oscillations are observed [22, 27, 33]. In this case, the screening factor behaves as $|x|^{-r} f(|x|)$, where $f: \mathbb{R}_{\geq 0} \rightarrow [-1, 1]$ is an oscillating function and the decay rate $r > 0$ depends on the Fermi surface of the metal. The *generic* exponential screening factor in (4.6) demonstrates that the TFW model significantly overscreens charges. \square

4.3. Neutrality of Defects

An immediate consequence of Corollary 4.1 is the neutrality of nuclear perturbations in the TFW equations. This result applies to all nuclear configurations belonging to $\mathcal{M}_{L^2}(M, \omega)$. In particular Theorem 4.1(3) strengthens the result of [10], which requires $m_1 - m_2 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ and thus excludes typical point defects; see Remark 8 for more details.

Theorem 4.1. *Let $m_1, m_2 \in \mathcal{M}_{L^2}(M, \omega)$ and define $\rho_{12} := m_1 - u_1^2 - m_2 + u_2^2$.*

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

$$\left| \int_{B_R(0)} \rho_{12} \right| \leq C e^{-\gamma R}. \quad (4.9)$$

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

$$\left| \int_{B_R(0)} \rho_{12} \right| \leq C(1 + R)^{2-r}. \quad (4.10)$$

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

$$\lim_{\varepsilon \rightarrow 0} \frac{1}{|B_\varepsilon(0)|} \int_{B_\varepsilon(0)} \widehat{\rho}_{12}(k) \, dk = 0, \quad (4.11)$$

where $\widehat{\rho}_{12}$ denotes the Fourier transform of ρ_{12} .

Remark 8. In a forthcoming article [13], we construct a variational problem to study the response of a crystal due to a local defect, using the TFW energy. Arguing as in [19], we shall show that any minimising displacement decays away from the defect at the rate $|x|^{-2}$, which corresponds to case (2) with $r = 2$. In this case (4.10) only provides a uniform bound for the charge as opposed to a decay estimate. However, as $r > 3/2$ the global neutrality result (4.11) holds for the relaxed system.

The neutrality estimates of Theorem 4.1 strengthen those of [10] in the following ways. Firstly, our result considers a perturbation of a general nuclear arrangement as opposed to a perfect crystal. This allows us, in [13], to consider the response of extended defects such as dislocations. In addition, we only require that the nuclear perturbation belongs to $L^2(\mathbb{R}^3)$, which we prove rigorously in [13], whereas in [10] the nuclear defect is assumed to lie in $L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, which fails for typical point defects. \square

4.4. Energy Locality

We now show that the locality result, Theorem 3.2, can be used to describe the energy contribution of each individual nucleus. In effect, we will derive a *site energy potential* for the TFW model, which has the surprising consequence that, for the study of mechanical response, TFW can be treated as a classical short-ranged interatomic potential. Our result gives credence to the construction of interatomic potentials and the assumption of *strong locality* used in hybrid quantum mechanics/molecular mechanics (QM/MM) simulations [17].

Let $\eta \in C_c^\infty(B_{R_0}(0))$ 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

$$m_Y(x) = \sum_{j \in \mathbb{N}} \eta(x - Y_j). \quad (4.12)$$

A natural space of nuclear coordinates, related to the \mathcal{M}_{L^2} space is

$$\mathcal{B}_{L^2}(M, \omega) := \left\{ Y \in (\mathbb{R}^3)^\mathbb{N} \mid m_Y \in \mathcal{M}_{L^2}(M, \omega) \right\}. \quad (4.13)$$

This space contains many condensed phases, such as crystals containing point defects, dislocations and grain boundaries. It does not include arrangements with arbitrarily large voids such as surfaces or cracks. However, as the TFW model for surfaces has been established [7], it may be possible to obtain locality estimates for surfaces and cracks using the TFW model.

We remark that there exists $R' = R'(R_0, \omega) > 0$ such that for any $Y \subset \mathcal{Y}_{L^2}(M, \omega)$

$$\bigcup_{j \in \mathbb{N}} B_{R'}(Y_j) = \mathbb{R}^3. \quad (4.14)$$

For any $Y \in \mathcal{Y}_{L^2}(M, \omega)$ there exists a unique ground state (u, ϕ) corresponding to $m = m_Y$. Naively, we might define the energy stored in a region $\Omega \subset \mathbb{R}^3$ by

$$\int_{\Omega} |\nabla u|^2 + \int_{\Omega} u^{10/3} + \frac{1}{2} \int_{\Omega} \left((m - u^2) * \frac{1}{|\cdot|} \right) (m - u^2), \quad (4.15)$$

however, difficulties arise due to the fact that $(m - u^2) * \frac{1}{|\cdot|}$ is not well-defined. Instead, we give two alternative definitions for the energy density for an infinite system:

$$\mathcal{E}_1(Y; \cdot) := |\nabla u|^2 + u^{10/3} + \frac{1}{2} \phi \left(m - u^2 \right), \quad (4.16)$$

$$\mathcal{E}_2(Y; \cdot) := |\nabla u|^2 + u^{10/3} + \frac{1}{8\pi} |\nabla \phi|^2, \quad (4.17)$$

which both satisfy $\mathcal{E}_1(Y; \cdot), \mathcal{E}_2(Y; \cdot) \in L^1_{\text{unif}}(\mathbb{R}^3)$.

Suppose now that $\Omega \subset \mathbb{R}^3$ is a charge-neutral volume [44], that is, if n is the unit normal to $\partial\Omega$, then $\nabla \phi \cdot n = 0$ on $\partial\Omega$. Recalling from (2.6b) that

$$-\Delta \phi = 4\pi \left(m - u^2 \right)$$

we deduce that

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

and hence

$$\int_{\Omega} \mathcal{E}_1(Y; x) \, dx = \int_{\Omega} \mathcal{E}_2(Y; x) \, dx.$$

In particular, for finite neutral systems $m_{R_n} = m \cdot \chi_{B_{R_n}(0)}$, where $m \in \mathcal{M}_{L^2}(M, \omega)$ and (u_{R_n}, ϕ_{R_n}) denoting the corresponding solution, the following energies agree on $\Omega = \mathbb{R}^3$

$$\begin{aligned} & \int_{\mathbb{R}^3} \left(|\nabla u_{R_n}|^2 + u_{R_n}^{10/3} + \frac{1}{2} \left((m_{R_n} - u_{R_n}^2) * \frac{1}{|\cdot|} \right) (m_{R_n} - u_{R_n}^2) \right) \\ &= \int_{\mathbb{R}^3} \left(|\nabla u_{R_n}|^2 + u_{R_n}^{10/3} + \frac{1}{2} \phi_{R_n} (m_{R_n} - u_{R_n}^2) \right) \\ &= \int_{\mathbb{R}^3} \left(|\nabla u_{R_n}|^2 + u_{R_n}^{10/3} + \frac{1}{8\pi} |\nabla \phi_{R_n}|^2 \right). \end{aligned} \quad (4.18)$$

We prove this claim is in Remark 12 in Section 6. Thus, we have derived two energy densities, $\mathcal{E}_1, \mathcal{E}_2$, which are meaningful and well-defined also for infinite configurations.

In order to define site energies, we require a partition of \mathbb{R}^3 . For each $j \in \mathbb{N}$ let $\varphi_j(Y; \cdot) \in C^1(\mathbb{R}^3)$, $\varphi_j(Y; \cdot) \geq 0$ satisfying the following conditions: there exist $C, \tilde{\gamma} > 0$ such that for all $Y \in \mathcal{Y}_{L^2}(M, \omega)$

$$\sum_{j \in \mathbb{N}} \varphi_j(Y; x) = 1, \quad (4.19a)$$

$$|\varphi_j(Y; x)| \leq C e^{-\tilde{\gamma}|x-Y_j|}, \quad \text{and} \quad (4.19b)$$

$$\left| \frac{\partial \varphi_j}{\partial Y_k}(Y; x) \right| \leq C e^{-\tilde{\gamma}|x-Y_j|} e^{-\tilde{\gamma}|x-Y_k|}. \quad (4.19c)$$

We propose a canonical construction of such a partition in Remark 9 below.

Given a family of partition functions satisfying (4.19), we can define site energies

$$E_j^i(Y) = \int_{\mathbb{R}^3} \mathcal{E}_i(Y; x) \varphi_j(Y; x) dx, \quad (4.20)$$

for $i = 1, 2$. A consequence of Theorems 3.1 and 3.2 is that $E_j^i(Y)$ are *local*: their dependence on the environment of nuclei decays exponentially fast. This is made precise in the following theorem.

Theorem 4.2. *Let $i \in \{1, 2\}$, $Y \in \mathcal{Y}_{L^2}(M, \omega)$ and $\{\varphi_j | j \in \mathbb{N}\}$ satisfy (4.19). Then for every $k \in \mathbb{N}$, $\partial_{Y_k} E_j^i$ exists and satisfies*

$$\left| \frac{\partial E_j^i(Y)}{\partial Y_k} \right| \leq C e^{-\gamma|Y_j-Y_k|}, \quad (4.21)$$

where $C = C(M, \omega)$, $\gamma = \gamma(M, \omega) > 0$.

The derivative $\partial_{Y_k} E_j^i$ can be interpreted as the contribution of the atom at Y_k to the force on the nucleus at Y_j . In addition, we show in Section 6.4 that these site energies generate the correct total force

$$\sum_{j \in \mathbb{N}} \frac{\partial E_j^1(Y)}{\partial Y_k} = \sum_{j \in \mathbb{N}} \frac{\partial E_j^2(Y)}{\partial Y_k} = \int_{\mathbb{R}^3} \phi(x) \frac{\partial m_Y(x)}{\partial Y_k} dx. \quad (4.22)$$

Remark 9. Two further canonical requirements on a site energy potential are permutation and isometry (rotation and translation) invariance. This can be obtained as follows:

If the partition $(\varphi_j)_{j \in \mathbb{N}}$ is *permutation invariant*, that is, for any bijection $P : \mathbb{N} \rightarrow \mathbb{N}$, $Y \circ P = (Y_{Pj})_{j \in \mathbb{N}}$, we have

$$\varphi_j(Y \circ P; x) = \varphi_{Pj}(Y; x) \quad \forall j \in \mathbb{N} \quad x \in \mathbb{R}^3, \quad (4.23)$$

then so are the site energies,

$$E_j^i(Y \circ P) = E_j^i(Y).$$

If the partition is *isometry invariant*, that is, for any isometry $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$, $AY = (AY_j)_{j \in \mathbb{N}}$, we have

$$\varphi_j(AY; x) = \varphi_j(Y; A^{-1}x) \quad \forall j \in \mathbb{N}, \quad x \in \mathbb{R}^3, \quad (4.24)$$

then the site energies are also isometry invariant,

$$E_j^i(AY) = E_j^i(Y).$$

Both statements are proven in Lemma 6.8.

A canonical class of partitions satisfying (4.19) as well as (4.23), (4.24) can be constructed as follows: Let $\tilde{\varphi} \in C^1(\mathbb{R}^3)$, $\tilde{\varphi} \geq 0$, be radially symmetric and satisfy

$$|\tilde{\varphi}(x)| + |\nabla \tilde{\varphi}(x)| \leq C e^{-\tilde{\gamma}|x|}, \quad (4.25)$$

$$\tilde{\varphi}(x) \geq c > 0 \quad \text{on } B_{R'+1}(0). \quad (4.26)$$

For example, this holds for $\tilde{\varphi}(x) = e^{-\tilde{\gamma}|x|^2}$ and for standard mollifiers with sufficiently wide support.

Then, for $j \in \mathbb{N}$, we can define

$$\varphi_j(Y; x) = \frac{\tilde{\varphi}(x - Y_j)}{\sum_{j' \in \mathbb{N}} \tilde{\varphi}(x - Y_{j'})}. \quad (4.27)$$

It is easy to see that this class of functions are well-defined and satisfies all requirements. \square

Remark 10. Alternative constructions of energy partitions include Bader volumes and charge-neutral volumes [4,32,44]. Bader volumes partition space into regions such that the flux of the electron density on the boundary is zero, while charge-neutral volumes are defined so that each region has zero charge. The construction of these volumes is not unique, like our definition of a partition. Bader volumes were developed as a means to define atoms within molecules [4].

With this in mind, using a partition we may assign a portion of the electron density to each nucleus in the system. We refer to a nucleus paired with its associated partition of the electron density as an effective atom. Due to the screening that occurs in the TFW model, the interaction of two effective atoms decays exponentially as the distance between the nuclei grows. In comparison, the interaction of two neutral atoms separated by a sufficiently large distance r in the TF model has been shown to decay at the rate r^{-7} [9]. This suggests that due to the overscreening of the TFW model, the interaction of the effective atoms is considerably weaker than is realistic. However, for the purpose of simulating quantum systems, in particular applying the strong locality principle [17], the weak long-range interaction of the TFW model is a desirable property. \square

Remark 11. The estimate shown in Theorem 4.2 is a theoretical result which can be applied to simulate defective crystals, though we do not pursue this. Locality estimates have been established for the tight-binding model and subsequently used to construct QM/MM hybrid methods [14,15]. \square

5. Conclusion and Outlook

The two main results of this work, Theorems 3.1 and 3.2, are stability and exponential locality estimates for the TFW model, which apply to general condensed nuclear configurations.

We have demonstrated in Section 4 that it can be used to extend and strengthen a range of existing results on the TFW model. A particular strength of our results is that they apply to general nuclear configuration in $\mathcal{M}_{L^2}(M, \omega)$, whereas the previous analyses of the TFW model have focused on (near)-crystalline arrangements or the homogeneous electron gas. This generality will be valuable when exploring the consequences of our analysis for studying models for the mechanical response problem in [13], where we generalise [19] to electronic structure models.

A further application, that we will develop in a forthcoming work is a study of the Yukawa potential as a model approximation [36, Theorem 3.5]. Adapting Theorems 3.1 and 3.2 we can consider the difference between the Coulomb and Yukawa ground states for a given nuclear configuration and prove uniform error estimates in terms of the screening parameter in the Yukawa model.

Two key difficulties in the analysis of electronic structure models are (i) the exchange and correlation of electrons due to the antisymmetry of the electronic wavefunction; and (ii) the interaction of charged particles (positive nuclei and negative electrons) via the long-range Coulomb potential. Since the TFW model is orbital-free it does not account for (i), however it fully incorporates Coulomb interaction. In this regard it is perhaps surprising that the TFW model satisfies the extremely generic locality property we obtained in Theorems 3.1 and 3.2.

The Hartree–Fock and Kohn–Sham models take both effects into account and whether these models permit a similarly strong notion of locality is an open problem. It is clear, however, that such results cannot be obtained in the generality that we considered in the present paper. Since charged defects exist in the reduced Hartree–Fock model [11] and as locality implies neutrality, this suggests that a locality property cannot hold for general condensed phase arrangements in the reduced Hartree–Fock model, which is the simplest model in the Hartree–Fock/Kohn–Sham class.

6. Proofs

This section contains the proofs of the main results. Proofs of results in Sections 3.1, 3.2 and 4 are found in Sections 6.1, 6.2 and 6.3 respectively.

The following is a preliminary result used in the construction of the space $\mathcal{M}_{L^2}(M, \omega)$.

Lemma 6.1. *Suppose $m : \mathbb{R}^3 \rightarrow \mathbb{R}_{\geq 0}$ and $m \in L^1_{\text{loc}}(\mathbb{R}^3)$, then (H2) is equivalent to the following statement: there exist $\omega_0, \omega_1 > 0$ such that for all $R > 0$*

$$\inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m(z) \, dz \geq \omega_0 R^3 - \omega_1. \quad (6.1)$$

Proof (Proof of Lemma 6.1). Clearly, (6.1) implies (H2), so suppose m satisfies (H2), then there exists $R_1 > 0$ such that

$$\inf_{x \in \mathbb{R}^3} \int_{B_{R_1}(x)} m(z) \, dz \geq 1.$$

For $R > 0$ and $x' \in \mathbb{R}^3$, let $Q_R(x') \subset \mathbb{R}^3$ denote the cube of side length $2R$ centred at x' , which contains $B_R(x')$. Also, let $R_2 = \sqrt{3}R_1$, which ensures that $B_{R_2}(x) \supset Q_{R_1}(x)$ for all $x \in \mathbb{R}^3$. Further, let $R \geq R_2$, hence $R = kR_2$, for some $k \geq 1$. Then

$$\begin{aligned} \inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m(z) \, dz &= \inf_{x \in \mathbb{R}^3} \int_{B_{kR_2}(x)} m(z) \, dz \geq \inf_{x \in \mathbb{R}^3} \int_{Q_{kR_1}(x)} m(z) \, dz \\ &\geq [k]^3 \inf_{x' \in \mathbb{R}^3} \int_{Q_{R_1}(x')} m(z) \, dz \geq [k]^3 \\ &\geq \left(\frac{k}{2}\right)^3 = \frac{R^3}{8R_2^3} =: \omega_0 R^3. \end{aligned} \quad (6.2)$$

Now define $\omega_1 := \omega_0 R_2^3 \geq 0$, then it follows from (6.2) that (6.1) holds for all $R > 0$. \square

6.1. Proofs of Uniform Regularity Estimates

The following lemma features in the proofs of both the existence and uniqueness of the TFW equations and is found in [12].

Lemma 6.2. *Let $a \in H_{\text{loc}}^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, then define the elliptic operator $L = -\Delta + a$. Suppose that there exists $u \in H_{\text{loc}}^1(\mathbb{R}^3)$ satisfying $u > 0$ and $Lu = 0$ in distribution. Then, the operator L is non-negative, that is for all $\varphi \in H^1(\mathbb{R}^3)$*

$$\langle \varphi, L\varphi \rangle \geq 0. \quad (6.3)$$

The proof is shown in [12] but is included here for completeness.

Proof (Proof of Lemma 6.2). Let $R > 0$ and define $\Omega = B_R(0)$ and consider L as an operator on $L^2(\Omega)$ with domain $H^2(\Omega) \cap H_0^1(\Omega)$. Then L is a self-adjoint operator with compact resolvent hence has a purely discrete spectrum. Since $a \in H_{\text{loc}}^1(\mathbb{R}^3)$ it follows that the smallest eigenvalue $\lambda_1(\Omega)$ is simple and has a positive eigenfunction $v_\Omega \in H_0^1(\Omega)$ [23, Theorem 8.38]. In addition, by standard elliptic regularity $v_\Omega \in H^3(\Omega) \hookrightarrow C^{1,1/2}(\overline{\Omega})$ [20] and solves

$$(-\Delta + a)v_\Omega = \lambda_1(\Omega)v_\Omega.$$

Testing this equation with u and using integration by parts, we obtain

$$-\int_{\partial\Omega} \frac{\partial v_\Omega}{\partial n} u = \lambda_1(\Omega) \int_{\Omega} v_\Omega u. \quad (6.4)$$

As $v_\Omega > 0$ on Ω and v_Ω vanishes over $\partial\Omega$, it follows that $\frac{\partial v_\Omega}{\partial n} \leq 0$. It follows that the left-hand side of (6.4) is non-negative, hence $\lambda_1(\Omega) \geq 0$. As this holds for $\Omega = B_R(0)$, for any $R > 0$, we deduce that for all $\varphi \in C_c^1(\mathbb{R}^3)$ $\langle \varphi, L\varphi \rangle \geq 0$. Using that $a \in L^\infty(\mathbb{R}^3)$ and the density of $C_c^1(\mathbb{R}^3)$ in $H^1(\mathbb{R}^3)$, it follows that for all $\varphi \in H^1(\mathbb{R}^3)$ $\langle \varphi, L\varphi \rangle \geq 0$. \square

We now show uniform estimates for finite systems corresponding to truncated nuclear distributions. This result is essentially [12, Proposition 3.5], however as we require uniform regularity estimates, we provide a complete proof.

Proposition 6.1. *Let $m : \mathbb{R} \rightarrow \mathbb{R}_{\geq 0}$ satisfy*

$$\|m\|_{L^2_{\text{unif}}(\mathbb{R}^3)} \leq M, \quad (6.5)$$

and $R_n \uparrow \infty$, then define the truncated nuclear distribution $m_{R_n} = m \cdot \chi_{B_{R_n}(0)}$. The unique solution to the minimisation problem

$$I^{\text{TFW}}(m_{R_n}) = \inf \left\{ E^{\text{TFW}}(v, m_{R_n}) \mid v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_{R_n} \right\},$$

yields a unique solution (u_{R_n}, ϕ_{R_n}) to (2.4)

$$\begin{aligned} -\Delta u_{R_n} + \frac{5}{3} u_{R_n}^{7/3} - \phi_{R_n} u_{R_n} &= 0, \\ -\Delta \phi_{R_n} &= 4\pi (m_{R_n} - u_{R_n}^2). \end{aligned}$$

which satisfy the following estimates, with constant C independent of R_n :

$$\|u_{R_n}\|_{H^4_{\text{unif}}(\mathbb{R}^3)} \leq C (1 + M^{15/4}), \quad (6.7)$$

$$\|\phi_{R_n}\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \leq C (1 + M^{3/2}). \quad (6.8)$$

Proof (Proof of Proposition 6.1). If $m \equiv 0$, then for all R_n , clearly $u_{R_n} = \phi_{R_n} = m_{R_n} = 0$ satisfies (2.4) and (6.7)–(6.8).

If $m \not\equiv 0$, then there exists a constant $R_0 \geq 0$ such that $R_n \geq R_0$ ensures that $\int_{\mathbb{R}^3} m_{R_n} > 0$. Recall

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

For each R_n , consider the minimisation problem

$$I^{\text{TFW}}(m_{R_n}) = \inf \left\{ E^{\text{TFW}}(v, m_{R_n}) \mid v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_{R_n} > 0 \right\}.$$

The constraint $\int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_{R_n}$ ensures the system is charge neutral, and by [31, Theorem 7.19] there exists a unique non-negative minimiser $u_{R_n} \in H^1(\mathbb{R}^3)$ to $I^{\text{TFW}}(m_{R_n})$ solving

$$-\Delta u_{R_n} + \frac{5}{3} u_{R_n}^{7/3} - \left((m_{R_n} - u_{R_n}^2) * \frac{1}{|\cdot|} \right) u_{R_n} = -\theta_{R_n} u_{R_n}, \quad (6.9)$$

$$\int_{\mathbb{R}^3} u_{R_n}^2 = \int_{\mathbb{R}^3} m_{R_n} > 0. \quad (6.10)$$

Here $\theta_{R_n} > 0$ is the Lagrange multiplier associated with the charge constraint (6.10) [12, 31]. Define $\phi_{R_n} : \mathbb{R}^3 \rightarrow \mathbb{R}$ by

$$\phi_{R_n} = \left((m_{R_n} - u_{R_n}^2) * \frac{1}{|\cdot|} \right) - \theta_{R_n}, \quad (6.11)$$

so we can express (6.9) as the Schrödinger–Poisson system (2.4)

$$\begin{aligned} -\Delta u_{R_n} + \frac{5}{3} u_{R_n}^{7/3} - \phi_{R_n} u_{R_n} &= 0, \\ -\Delta \phi_{R_n} &= 4\pi (m_{R_n} - u_{R_n}^2). \end{aligned}$$

Decompose

$$(m_{R_n} - u_{R_n}^2) * \frac{1}{|\cdot|} = (m_{R_n} - u_{R_n}^2) * \left(\frac{1}{|\cdot|} \chi_{B_1(0)} \right) + (m_{R_n} - u_{R_n}^2) * \left(\frac{1}{|\cdot|} \chi_{B_1(0)^c} \right),$$

then as $u_{R_n} \in H^1(\mathbb{R}^3) \hookrightarrow L^6(\mathbb{R}^3)$ and $m \in L^2_{\text{unif}}(\mathbb{R}^3)$ applying Young's inequality gives

$$\begin{aligned} \left\| (m_{R_n} - u_{R_n}^2) * \frac{1}{|\cdot|} \right\|_{L^\infty(\mathbb{R}^3)} &\leq \left\| (m_{R_n} - u_{R_n}^2) \right\|_{L^{5/3}(\mathbb{R}^3)} \left\| \frac{1}{|\cdot|} \chi_{B_1(0)} \right\|_{L^{5/2}(\mathbb{R}^3)} \\ &\quad + \left\| (m_{R_n} - u_{R_n}^2) \right\|_{L^{7/5}(\mathbb{R}^3)} \left\| \frac{1}{|\cdot|} \chi_{B_1(0)^c} \right\|_{L^{7/2}(\mathbb{R}^3)} \\ &\leq C \left((R_n^{3/10} + R_n^{9/14}) \|m_{R_n}\|_{L^2(\mathbb{R}^3)} + \|u_{R_n}\|_{H^1(\mathbb{R}^3)}^2 \right) \\ &\leq C \left((R_n^{9/5} + R_n^{15/7}) \|m\|_{L^2_{\text{unif}}(\mathbb{R}^3)} + \|u_{R_n}\|_{H^1(\mathbb{R}^3)}^2 \right) \\ &\leq C \left((R_n^{9/5} + R_n^{15/7}) M + \|u_{R_n}\|_{H^1(\mathbb{R}^3)}^2 \right). \end{aligned}$$

By [30, Lemma II.25] we deduce that $(m_{R_n} - u_{R_n}^2) * \frac{1}{|\cdot|}$ is a continuous function vanishing at infinity. It follows that $\phi_{R_n} \in L^\infty(\mathbb{R}^3)$ and is also continuous. Also, $|\nabla \phi_{R_n}| \in L^2(\mathbb{R}^3)$

$$\begin{aligned} \frac{1}{8\pi} \int_{\mathbb{R}^3} |\nabla \phi_{R_n}|^2 &= \frac{1}{8\pi} \int_{\mathbb{R}^3} \phi_{R_n} (-\Delta \phi_{R_n}) \\ &= \frac{1}{2} \int_{\mathbb{R}^3} \phi_{R_n} (m_{R_n} - u_{R_n}^2) \\ &= \frac{1}{2} \int_{\mathbb{R}^3} \phi_{R_n} (m_{R_n} - u_{R_n}^2) + \frac{\theta_{R_n}}{2} \int_{\mathbb{R}^3} (m_{R_n} - u_{R_n}^2) \\ &= \frac{1}{2} \int_{\mathbb{R}^3} (\phi_{R_n} + \theta_{R_n}) (m_{R_n} - u_{R_n}^2) \\ &= \frac{1}{2} \int_{\mathbb{R}^3} \left((m_{R_n} - u_{R_n}^2) * \frac{1}{|\cdot|} \right) (m_{R_n} - u_{R_n}^2), \end{aligned} \quad (6.12)$$

hence $\phi_{R_n} \in H^1_{\text{unif}}(\mathbb{R}^3)$. Now, consider $u_{R_n} \in H^1(\mathbb{R}^3)$, which solves

$$-\Delta u_{R_n} = -\frac{5}{3} u_{R_n}^{7/3} + \phi_{R_n} u_{R_n}. \quad (6.13)$$

The right-hand side can be estimated in $L^2(\mathbb{R}^3)$ by

$$\begin{aligned} \left\| \frac{5}{3} u_{R_n}^{7/3} - \phi_{R_n} u_{R_n} \right\|_{L^2(\mathbb{R}^3)} &\leq \frac{5}{3} \left\| u_{R_n}^{7/3} \right\|_{L^2(\mathbb{R}^3)} + \left\| \phi_{R_n} \right\|_{L^\infty(\mathbb{R}^3)} \left\| u_{R_n} \right\|_{L^2(\mathbb{R}^3)} \\ &\leq C \left\| u_{R_n} \right\|_{H^1(\mathbb{R}^3)}^{7/3} + \left\| \phi_{R_n} \right\|_{L^\infty(\mathbb{R}^3)} \left\| u_{R_n} \right\|_{H^1(\mathbb{R}^3)}, \end{aligned}$$

which implies $u_{R_n} \in H^2(\mathbb{R}^3)$ as $\Delta u_{R_n} \in L^2(\mathbb{R}^3)$. By the Sobolev Embedding Theorem [20] $u_{R_n} \in H^2(\mathbb{R}^3) \hookrightarrow C^{0,1/2}(\mathbb{R}^3)$, hence u_{R_n} is continuous. Also, by [5, Lemma 9], u_{R_n} decays at infinity. We now justify this. Recall (6.13) and since $u_{R_n} \geq 0$, we have $-\Delta u_{R_n} \leq \phi_{R_n} u_{R_n}$, hence

$$-\Delta u_{R_n} + u_{R_n} \leq (1 + \phi_{R_n}) u_{R_n}$$

As $\phi_{R_n} \in L^\infty(\mathbb{R}^3)$ and $u_{R_n} \in H^1(\mathbb{R}^3)$, the right-hand side belongs to $L^2(\mathbb{R}^3)$ hence by the Lax–Milgram theorem there exists a unique $g_{R_n} \in H^1(\mathbb{R}^3)$ satisfying

$$-\Delta g_{R_n} + g_{R_n} = (1 + \phi_{R_n}) u_{R_n}.$$

Moreover, using the Green’s function $g_{R_n} = \frac{e^{-|\cdot|}}{|\cdot|} * (1 + \phi_{R_n}) u_{R_n}$ and since $\frac{e^{-|\cdot|}}{|\cdot|}, (1 + \phi_{R_n}) u_{R_n} \in L^2(\mathbb{R}^3)$ by [30, Lemma II.25] g_{R_n} is continuous function that decays at infinity, hence $g_{R_n} \in L^\infty(\mathbb{R}^3)$. It follows from the comparison principle that $u_{R_n} \leq g_{R_n}$, so $u_{R_n} \in L^\infty(\mathbb{R}^3)$ and decays at infinity.

Using that $u_{R_n}, \phi_{R_n} + \theta_{R_n}$ are continuous and decay at infinity, by arguing as in [41], there exists a universal constant $C_S > 0$, independent of the nuclear distribution, satisfying

$$0 < \theta_{R_n} \leq C_S, \quad (6.14)$$

$$\frac{10}{9} u_{R_n}^{4/3} \leq \phi_{R_n} + C_S. \quad (6.15)$$

As $u_{R_n} \geq 0$, from the Solovej estimate (6.15) we obtain the uniform lower bound

$$\phi_{R_n} \geq -C_S. \quad (6.16)$$

We aim to show a uniform upper bound for ϕ_{R_n} , which together with (6.15) will yield the uniform estimate

$$\left\| u_{R_n} \right\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \left\| \phi_{R_n} \right\|_{L^\infty(\mathbb{R}^3)} \leq C(M), \quad (6.17)$$

which is independent of R_n .

If ϕ_{R_n} is non-positive, then (6.17) holds as

$$\left\| u_{R_n} \right\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \left\| \phi_{R_n} \right\|_{L^\infty(\mathbb{R}^3)} \leq 2C_S.$$

Instead, suppose that $\phi_{R_n}^+$ is non-zero at some point in \mathbb{R}^3 . By (6.11) ϕ_{R_n} is a continuous function that converges to a negative limit at infinity, $\phi_{R_n}^+ \in C_c(\mathbb{R}^3)$, hence there exists a point $x_{R_n} \in \mathbb{R}^3$ such that

$$\phi_{R_n}^+(x_{R_n}) = \left\| \phi_{R_n}^+ \right\|_{L^\infty(\mathbb{R}^3)} > 0. \quad (6.18)$$

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

We now show that $u_{R_n} > 0$ on \mathbb{R}^3 , arguing by contradiction. Suppose that there exists $z \in \mathbb{R}^3$ such that $u_{R_n}(z) = 0$. Since u_{R_n} is a non-negative, continuous function decaying at infinity, there exists $y_n \in \mathbb{R}^3$ such that

$$u_{R_n}(y_n) = \sup_{x \in \mathbb{R}^3} u_{R_n}(x).$$

Let $R > |y_n - z|$, then by the Harnack inequality [42], we infer

$$0 \leq u_{R_n}(y_n) = \sup_{x \in B_R(y_n)} u_{R_n}(x) \leq C(R) \inf_{x \in B_R(y_n)} u_{R_n}(x) = u_{R_n}(z) = 0,$$

so $u_{R_n} \equiv 0$. This contradicts the charge constraint (6.10) $\int_{\mathbb{R}^3} u_{R_n}^2 = \int_{\mathbb{R}^3} m_{R_n} > 0$, hence $u_{R_n} > 0$ on \mathbb{R}^3 .

As $u_{R_n} \in H^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, $\phi_{R_n} \in H_{\text{unif}}^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ and $u_{R_n} > 0$, Lemma 6.2 implies that $L_{R_n} = -\Delta + \frac{5}{3}u_{R_n}^{4/3} - \phi_{R_n}$ is a non-negative operator.

Choose $\varphi \in C_c^\infty(B_1(0))$ satisfying $0 \leq \varphi \leq 1$, $\varphi = 1$ on $B_{1/2}(0)$, $\int_{\mathbb{R}^3} \varphi^2 = 1$ and $\int_{\mathbb{R}^3} |\nabla \varphi|^2 =: c_\varphi$, 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_{R_n} is non-negative (6.3) implies

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

which can be re-arranged and expressed using convolutions as

$$\begin{aligned} \frac{5}{3} \left(u_{R_n}^{4/3} * \varphi^2 \right) &\geq \left(\phi_{R_n} * \varphi^2 - \int_{\mathbb{R}^3} |\nabla \varphi|^2 \right)_+ \\ &= \left(\phi_{R_n} * \varphi^2 - c_\varphi \right)_+ \end{aligned} \quad (6.19)$$

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

$$-\Delta \left(\phi_{R_n} * \varphi^2 \right) = 4\pi \left(m_{R_n} * \varphi^2 - u_{R_n}^2 * \varphi^2 \right). \quad (6.20)$$

We estimate the first term using (6.5)

$$\begin{aligned} \left(m_{R_n} * \varphi^2 \right)(x) &= \int_{B_1(x)} m_{R_n}(y) \varphi^2(x - y) \, dy \\ &\leq \int_{B_1(x)} m(y) \, dy \leq C_0 \|m\|_{L_{\text{unif}}^2(\mathbb{R}^3)} \leq C_0 M. \end{aligned} \quad (6.21)$$

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 (6.19) we deduce

$$\begin{aligned}
 4\pi u_{R_n}^2 * \varphi^2(x) &\geq \frac{5}{3} u_{R_n}^2 * \varphi^2(x) \\
 &= \frac{5}{3} \int_{\mathbb{R}^3} u_{R_n}^2(x-y) \varphi^2(y) \, dy \\
 &= \frac{5}{3} \int_{\mathbb{R}^3} \left(u_{R_n}^{4/3}(x-y) \right)^{3/2} \varphi^2(y) \, dy \\
 &\geq \frac{5}{3} \left(\int_{\mathbb{R}^3} u_{R_n}^{4/3}(x-y) \varphi^2(y) \, dy \right)^{3/2} \\
 &= \frac{5}{3} \left(u_{R_n}^{4/3} * \varphi^2 \right)^{3/2} \geq \left(\phi_{R_n} * \varphi^2 - c_\varphi \right)_+^{3/2}. \quad (6.22)
 \end{aligned}$$

Combining the estimates (6.20)–(6.22) we conclude that

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

By (6.11), as ϕ_{R_n} is a continuous function that converges to a negative limit at infinity, $\phi_{R_n} * \varphi^2$ also shares these properties. Now consider the set

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

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

$$\begin{aligned}
 -\Delta h + h_+^{3/2} &= C_0 M \quad \text{on } S, \\
 0 &= \phi_{R_n} * \varphi^2 - c_\varphi \leq h \quad \text{in } \partial S,
 \end{aligned}$$

so by the maximum principle $\phi_{R_n} * \varphi^2 \leq c_\varphi + C_0^{2/3} M^{2/3}$ over S , and also on S^c , hence

$$\phi_{R_n} * \varphi^2 \leq C_1 \left(1 + M^{2/3} \right), \quad (6.23)$$

where $C_1 = \max\{c_\varphi, C_0^{2/3}\}$ is independent of M .

Observe that

$$\phi_{R_n}^+ * \varphi^2 = \phi_{R_n}^- * \varphi^2 + \phi_{R_n} * \varphi^2 \leq C_S + C_1 \left(1 + M^{2/3} \right) = C \left(1 + M^{2/3} \right),$$

and by estimating (2.4b) directly, that

$$-\Delta \phi_{R_n}^+ = -\Delta \phi_{R_n} \chi_{\{\phi_{R_n} > 0\}} = 4\pi \left(m_{R_n} - u_{R_n}^2 \right) \chi_{\{\phi_{R_n} > 0\}} \leq 4\pi m_{R_n} \chi_{\{\phi_{R_n} > 0\}} \leq 4\pi m_{R_n}.$$

As $0 \leq \varphi \leq 1$ and $\varphi = 1$ on $B_{1/2}(0)$, then

$$\int_{B_{1/2}(0)} \phi_{R_n}^+(x) \, dx \leq \left(\phi_{R_n}^+ * \varphi^2 \right)(0) \leq C \left(1 + M^{2/3} \right). \quad (6.24)$$

Using a change of variables, (6.24) can be expressed as

$$\int_{B_{1/2}(0)} \phi_{R_n}^+(x) \, dx = \int_0^{1/2} \int_{S_t(0)} \phi_{R_n}^+(t\gamma) \, dS_t(\gamma) \, dt.$$

Define $f : [0, 1/2] \rightarrow \mathbb{R}$ by

$$f(t) = \int_{S_t(0)} \phi_{R_n}^+(t\gamma) \, dS_t(\gamma)$$

and suppose that for all $t \in (1/4, 1/2)$

$$f(t) > 4 \int_{B_{1/2}(0)} \phi_{R_n}^+(x) \, dx > 0,$$

then

$$\int_{B_{1/2}(0)} \phi_{R_n}^+(x) \, dx = \int_0^{1/2} f(t) \, dt \geq \int_{1/4}^{1/2} f(t) \, dt > \int_{B_{1/2}(0)} \phi_{R_n}^+(x) \, dx,$$

which gives a contradiction, hence for some $t \in (1/4, 1/2)$

$$\int_{S_t(0)} \phi_{R_n}^+(t\gamma) \, dS_t(\gamma) \leq 4 \int_{B_{1/2}(0)} \phi_{R_n}^+(x) \, dx \leq C \left(1 + M^{2/3}\right). \quad (6.25)$$

Since $t > 1/4$, (6.25) implies

$$\begin{aligned} \int_{S_t(0)} \phi_{R_n}^+(t\gamma) \, dS_t(\gamma) &= \frac{1}{|S_t(0)|} \int_{S_t(0)} \phi_{R_n}^+(t\gamma) \, dS_t(\gamma) \\ &\leq \frac{C + M^{2/3}}{|S_{1/4}(0)|} \leq C \left(1 + M^{2/3}\right) =: C_1(M). \end{aligned}$$

We now construct an upper bound for $\phi_{R_n}^+$ as follows. Let ϕ_1 satisfy

$$\begin{aligned} -\Delta \phi_1 &= 0 && \text{in } B_t(0), \\ \phi_1 &= \phi_{R_n}^+ && \text{on } S_t(0). \end{aligned}$$

As ϕ_1 is harmonic, it satisfies the mean value property

$$\phi_1(0) \leq \int_{S_t(0)} \phi_{R_n}^+(t\gamma) \, dS_t(\gamma) \leq C_1(M). \quad (6.26)$$

Then consider the Dirichlet problem

$$\begin{aligned} -\Delta \phi_2 &= 4\pi m && \text{in } B_t(0), \\ \phi_2 &= 0 && \text{on } S_t(0). \end{aligned}$$

By Lax-Milgram, this has a unique weak solution $\phi_2 \in H_0^1(B_t(0))$. By standard elliptic regularity theory [20] $\phi_2 \in H^2(B_t(0)) \hookrightarrow C^{0,1/2}(\overline{B_t(0)})$ and

$$\|\phi_2\|_{C^{0,1/2}(\overline{B_t(0)})} \leq C \|\phi_2\|_{H^2(B_t(0))} \leq C \|m\|_{L^2(B_t(0))} \leq C t^{3/2} \|m\|_{L_{\text{unif}}^2(\mathbb{R}^3)} \leq CM. \quad (6.27)$$

The constructed functions ϕ_1, ϕ_2 satisfy

$$\begin{aligned} -\Delta\phi_{R_n}^+ &\leq -\Delta(\phi_1 + \phi_2) \quad \text{in } B_t(0), \\ \phi_{R_n}^+ &= \phi_1 + \phi_2 \quad \text{on } S_t(0), \end{aligned}$$

hence by the maximum principle $\phi_{R_n}^+ \leq \phi_1 + \phi_2$, in particular (6.26)–(6.27) imply

$$\|\phi_{R_n}^+\|_{L^\infty(\mathbb{R}^3)} = \phi_{R_n}^+(0) \leq \phi_1(0) + \phi_2(0) \leq C(1 + M),$$

where the right-hand side is independent of R_n . Combining this with the lower bound (6.16) and the Solovej estimate (6.15), we obtain the estimate (6.17)

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

It follows immediately that for all $x \in \mathbb{R}^3$ and $r \in [1, \infty]$

$$\|u_{R_n}\|_{L^r(B_2(x))} \leq C \left(1 + M^{3/4}\right), \quad (6.28)$$

independently of both x, r and R_n . Using (6.17) and (6.28), we now obtain uniform local estimates for the right-hand side of (6.13)

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

by

$$\begin{aligned} \left\| \frac{5}{3}u_{R_n}^{7/3} - \phi_{R_n}u_{R_n} \right\|_{L^2(B_2(x))} &\leq C \left\| \frac{5}{3}u_{R_n}^{7/3} - \phi_{R_n}u_{R_n} \right\|_{L^\infty(\mathbb{R}^3)} \\ &\leq C \left(\|u_{R_n}\|_{L^\infty(\mathbb{R}^3)}^{7/3} + \|\phi_{R_n}\|_{L^\infty(\mathbb{R}^3)} \|u_{R_n}\|_{L^\infty(\mathbb{R}^3)} \right) \\ &\leq C \left(1 + M^{7/4}\right). \end{aligned}$$

Consequently, for any $x \in \mathbb{R}^3$, the elliptic regularity estimate [20] gives

$$\begin{aligned} \|u_{R_n}\|_{H^2(B_1(x))} &\leq C \left(\left\| \frac{5}{3}u_{R_n}^{7/3} - \phi_{R_n}u_{R_n} \right\|_{L^2(B_2(x))} + \|u_{R_n}\|_{L^2(B_2(x))} \right) \\ &\leq C(1 + M^{7/4}) + C \left(1 + M^{1/2}\right) \leq C \left(1 + M^{7/4}\right). \end{aligned} \quad (6.29)$$

As (6.29) is independent of $x \in \mathbb{R}^3$, we obtain

$$\|u_{R_n}\|_{H_{\text{unif}}^2(\mathbb{R}^3)} \leq C \left(1 + M^{7/4}\right). \quad (6.30)$$

Applying a similar argument to estimate the right-hand side of (2.4b)

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

yields (6.8)

$$\|\phi_{R_n}\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \leq C \left(1 + M^{3/2}\right).$$

Using that $\phi_{R_n} \in H^2_{\text{unif}}(\mathbb{R}^3)$ and arguing as in (6.30), we obtain the desired estimate (6.7)

$$\|u_{R_n}\|_{H^4_{\text{unif}}(\mathbb{R}^3)} \leq C \left(1 + M^{15/4}\right).$$

We remark that while the constants appearing in the final estimates (6.7)–(6.8) depend on c_φ , they are independent of M . \square

Remark 12. We now justify the claim that for finite and neutral systems and for $\Omega = \mathbb{R}^3$, the three energies shown in (4.18) agree. Recall (6.12), which shows that the Coulomb energy can be expressed as

$$\begin{aligned} \frac{1}{2} \int_{\mathbb{R}^3} \left((m_{R_n} - u_{R_n}^2) * \frac{1}{|\cdot|} \right) (m_{R_n} - u_{R_n}^2) &= \frac{1}{2} \int_{\mathbb{R}^3} \phi_{R_n} (m_{R_n} - u_{R_n}^2) \\ &= \frac{1}{8\pi} \int_{\mathbb{R}^3} |\nabla \phi_{R_n}|^2, \end{aligned}$$

so it follows that the energies defined in (4.18) agree for $\Omega = \mathbb{R}^3$. \square

We now discuss passing to the limit in (2.4) to obtain regularity for the infinite system.

Proof (Proof of Proposition 3.1). First suppose that $\text{spt}(m)$ is bounded, then for sufficiently large R_n , $m = m_{R_n}$ and hence by Proposition 6.1 $(u, \phi) = (u_{R_n}, \phi_{R_n})$ solves (2.6) and satisfies the desired estimates (3.2)–(3.3).

Now suppose $\text{spt}(m)$ is unbounded, then the estimates (6.7)–(6.8) of Proposition 6.1 guarantee that the sequences u_{R_n}, ϕ_{R_n} are bounded uniformly in $H^2_{\text{unif}}(\mathbb{R}^3)$. Consequently, there exist $u, \phi \in H^2_{\text{unif}}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ such that along a subsequence u_{R_n}, ϕ_{R_n} converges to u, ϕ , 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 $u \geq 0$ and

$$\begin{aligned} \|u\|_{L^\infty(\mathbb{R}^3)} &\leq C \left(1 + M^{3/4}\right), \\ \|\phi\|_{L^\infty(\mathbb{R}^3)} &\leq C(1 + M). \end{aligned}$$

Passing to the limit of the equations (2.4) in distribution, we find that the limit (u, ϕ) solves

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

Arguing as in (6.7)–(6.8), we deduce that the desired estimates (3.2)–(3.3) hold

$$\begin{aligned} \|u\|_{H^4_{\text{unif}}(\mathbb{R}^3)} &\leq C \left(1 + M^{15/4}\right), \\ \|\phi\|_{H^2_{\text{unif}}(\mathbb{R}^3)} &\leq C \left(1 + M^{3/2}\right). \end{aligned}$$

\square

Proof (Proof of Proposition 3.2). As $m \in \mathcal{M}_{L^2}(M, \omega)$, it satisfies (H1)–(H2), hence by Theorem 2.1, the solution (u, ϕ) of (2.6) defined in Proposition 3.1 is unique and satisfies $\inf u > 0$. Now suppose

$$\inf_{m \in \mathcal{M}_{L^2}(M, \omega)} \inf_{x \in \mathbb{R}^3} u(x) = 0, \quad (6.31)$$

we show that this contradicts the assumption that for all $m \in \mathcal{M}_{L^2}(M, \omega)$ and $R > 0$

$$\inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m(z) \, dz \geq \omega_0 R^3 - \omega_1.$$

It follows from (6.31) that there exists $m_n \in \mathcal{M}_{L^2}(M, \omega)$ with corresponding solution (u_n, ϕ_n) and $x_n \in \mathbb{R}^3$ such that for all $n \in \mathbb{N}$

$$u_n(x_n) \leq \frac{1}{n}.$$

Recall the uniform estimates (6.7)–(6.8) from Proposition 3.1

$$\begin{aligned} \|u_n\|_{H_{\text{unif}}^4(\mathbb{R}^3)} &\leq C \left(1 + M^{15/4}\right), \\ \|\phi_n\|_{H_{\text{unif}}^2(\mathbb{R}^3)} &\leq C \left(1 + M^{3/2}\right). \end{aligned}$$

It follows that

$$\left\| \frac{5}{3} u_n^{4/3} - \phi_n u_n \right\|_{L_{\text{unif}}^2(\mathbb{R}^3)} \leq C \|u_n\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \|\phi_n\|_{L_{\text{unif}}^2(\mathbb{R}^3)} \|u_n\|_{L^\infty(\mathbb{R}^3)} \leq C(M).$$

As $\frac{5}{3} u_n^{4/3} - \phi_n u_n \in L_{\text{loc}}^2(\mathbb{R}^3)$, $u_n \in H_{\text{unif}}^1(\mathbb{R}^3)$ 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 [42], 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 $C = C(R, M) > 0$ such that

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

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 .

Recall that ϕ_n solves the following equation in distribution

$$-\Delta \phi_n = 4\pi \left(m_n - u_n^2 \right). \quad (6.32)$$

We translate the system and then pass to the limit in (6.32) as n tends to infinity. To do this, we use the following estimates, which are translation invariant:

$$\begin{aligned}\|m_n(\cdot + x_n)\|_{L^2_{\text{unif}}(\mathbb{R}^3)} &\leq M, \\ \|\phi_n(\cdot + x_n)\|_{H^2_{\text{unif}}(\mathbb{R}^3)} &\leq C(M).\end{aligned}$$

It follows that, up to a subsequence, $\phi_n(\cdot + x_n)$ converges to $\tilde{\phi}$, weakly in $H^2(B_R(0))$, strongly in $H^1(B_R(0))$ for all $R > 0$ and pointwise almost everywhere. Moreover, $m_n(\cdot + x_n)$ converges to \tilde{m} , weakly in $L^2(B_R(0))$ for all $R > 0$. By applying the Lebesgue–Besicovitch Differentiation Theorem [21] we deduce that $\tilde{m} \in \mathcal{M}_{L^2}(M, \omega)$. Passing to the limit in

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

it follows that $\tilde{\phi}$ is a distributional solution of

$$-\Delta\tilde{\phi} = 4\pi\tilde{m}. \quad (6.33)$$

Arguing as in [12, Theorem 6.10], we show that for all $R > 0$

$$\int_{B_R(0)} \tilde{m}(z) \, dz \leq CR. \quad (6.34)$$

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

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

To show (6.34) 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 (6.33) with $\varphi(\cdot/R)$ gives

$$-\frac{1}{R^2} \int_{B_{2R}(0)} \tilde{\phi}(z) (\Delta\varphi)(z/R) \, dz = 4\pi \int_{B_{2R}(0)} \tilde{m}(z) \varphi(z/R) \, dz. \quad (6.35)$$

The left-hand side can be estimated by

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

where the constant $C > 0$ is independent of R . As $\tilde{m} \geq 0$, from (6.35) we obtain (6.34)

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

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

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

□

Proof (Proof of Corollary 3.1). Our aim is to show by induction that for all $k \in \mathbb{N}_0$, if $m \in \mathcal{M}_{H^k}(M, \omega)$ then the corresponding solution (u, ϕ) to (2.6) satisfies

$$\|u\|_{H_{\text{unif}}^{k+4}(\mathbb{R}^3)} + \|\phi\|_{H_{\text{unif}}^{k+2}(\mathbb{R}^3)} \leq C(k, M, \omega). \quad (6.36)$$

In Proposition 3.1, by combining the estimates (3.2) and (3.3), it follows that (6.36) holds for the case $k = 0$: for all $m \in \mathcal{M}_{L^2}(M, \omega)$ the corresponding solution (u, ϕ) satisfies

$$\|u\|_{H_{\text{unif}}^4(\mathbb{R}^3)} + \|\phi\|_{H_{\text{unif}}^2(\mathbb{R}^3)} \leq C(M, \omega).$$

We now show the induction step. Suppose the result is true for $k \in \mathbb{N}_0$, then consider $m \in \mathcal{M}_{H^{k+1}}(M, \omega) \subset \mathcal{M}_{H^k}(M, \omega)$, so by the induction hypothesis the corresponding solution (u, ϕ) satisfies

$$\|u\|_{H_{\text{unif}}^{k+4}(\mathbb{R}^3)} + \|\phi\|_{H_{\text{unif}}^{k+2}(\mathbb{R}^3)} \leq C\left(k, \|m\|_{H_{\text{unif}}^k(\mathbb{R}^3)}, \omega\right). \quad (6.37)$$

We remark that as $0 < c_{M, \omega} \leq u \leq C(M)$ and $u \in H_{\text{unif}}^{k+4}(\mathbb{R}^3)$, it follows that for all $r \in \mathbb{R}$, $u^r \in H_{\text{unif}}^{k+4}(\mathbb{R}^3)$. As (u, ϕ) solve (2.6)

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

by standard elliptic regularity theory [20] for any $x \in \mathbb{R}^3$

$$\begin{aligned} \|\phi\|_{H^{k+3}(B_1(x))} &\leq C\left(\|m - u^2\|_{H^{k+1}(B_2(x))} + \|\phi\|_{L^2(B_2(x))}\right) \\ &\leq C\left(\|m\|_{H^{k+1}(B_2(x))} + \|u^2\|_{H^{k+1}(B_2(x))} + \|\phi\|_{L^2(B_2(x))}\right) \\ &\leq C\left(\|m\|_{H_{\text{unif}}^{k+1}(\mathbb{R}^3)} + \|\phi\|_{L_{\text{unif}}^2(\mathbb{R}^3)}\right) + C\left(k+1, \|u\|_{H_{\text{unif}}^{k+1}(\mathbb{R}^3)}\right) \\ &\leq C\|m\|_{H_{\text{unif}}^{k+1}(\mathbb{R}^3)} + C\left(k+1, \|m\|_{H_{\text{unif}}^k(\mathbb{R}^3)}, \omega\right) \\ &\leq C\left(k+1, \|m\|_{H_{\text{unif}}^{k+1}(\mathbb{R}^3)}, \omega\right), \end{aligned}$$

hence

$$\|\phi\|_{H_{\text{unif}}^{k+3}(\mathbb{R}^3)} = \sup_{x \in \mathbb{R}^3} \|\phi\|_{H^{k+3}(B_1(x))} \leq C\left(k+1, \|m\|_{H_{\text{unif}}^{k+1}(\mathbb{R}^3)}, \omega\right). \quad (6.38)$$

We use an identical argument together and apply the estimate (6.38) to deduce

$$\begin{aligned} \|u\|_{H_{\text{unif}}^{k+5}(\mathbb{R}^3)} &\leq C\left(\left\|\frac{5}{3}u^{7/3} - \phi u\right\|_{H_{\text{unif}}^{k+3}(\mathbb{R}^3)} + \|u\|_{L_{\text{unif}}^2(\mathbb{R}^3)}\right) \\ &\leq C\left(\|\phi\|_{H_{\text{unif}}^{k+3}(\mathbb{R}^3)}, \|u\|_{H_{\text{unif}}^{k+3}(\mathbb{R}^3)}\right) \\ &\leq C\left(k+1, \|m\|_{H_{\text{unif}}^{k+1}(\mathbb{R}^3)}, \omega\right). \end{aligned} \quad (6.39)$$

Combining (6.38) and (6.39) we obtain the desired estimate

$$\|u\|_{H_{\text{unif}}^{k+5}(\mathbb{R}^3)} + \|\phi\|_{H_{\text{unif}}^{k+3}(\mathbb{R}^3)} \leq C \left(k + 1, \|m\|_{H_{\text{unif}}^{k+1}(\mathbb{R}^3)}, \omega \right),$$

which completes the proof of (6.36) by induction. \square

6.2. Proofs of Pointwise Stability Estimates

To prove Theorems 3.1 and 3.2, we adapt the proof of uniqueness of the TFW equations, shown in [7, 12]. Due to the length of the argument, we shall prove several intermediate results. Before showing these results, we outline the structure of the proof.

First, we state two alternative sets of assumptions on nuclear distributions m_1, m_2 :

- (A) Let $k = 0$, $m_1 \in \mathcal{M}_{L^2}(M, \omega)$, and let (u_1, ϕ_1) denote the corresponding ground state. Also, let $m_2 : \mathbb{R}^3 \rightarrow \mathbb{R}_{\geq 0}$ satisfy $\|m_2\|_{L_{\text{unif}}^2(\mathbb{R}^3)} \leq M'$ and suppose there exists (u_2, ϕ_2) solving (2.6) corresponding to m_2 , satisfying $u_2 \geq 0$ and

$$\|u_2\|_{H_{\text{unif}}^4(\mathbb{R}^3)} + \|\phi_2\|_{H_{\text{unif}}^2(\mathbb{R}^3)} \leq C(M'). \quad (6.40)$$

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

- (B) Let $k \in \mathbb{N}_0$, $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$ and let $(u_1, \phi_1), (u_2, \phi_2)$ denote the corresponding ground states. (Note that (B) implies (A), with $M' = C(M)$.)

Remark 13. We point out that in (A) we assume $u_2 > 0$, while in Theorem 3.1 we only require $u_2 \geq 0$. The restriction $u_2 > 0$ allows us to directly use results from [12], in particular Lemma 6.2, and will be lifted via a thermodynamic limit argument in the third part of its proof on page 38. \square

Throughout the remainder of the paper we use the notation

$$w = u_1 - u_2, \quad \psi = \phi_1 - \phi_2, \quad R_m = 4\pi(m_1 - m_2).$$

By treating the coupled system of equations as a linear system and by exploiting the coupling between the electron density and electrostatic potential arising from the Coulomb energy term of the TFW functional, we obtain the following initial estimates

Lemma 6.3. Suppose (A) holds, then there exists $C = C(M, M', \omega) > 0$ such that for any $\xi \in H^1(\mathbb{R}^3)$

$$\int_{\mathbb{R}^3} \left(w^2 + |\nabla w|^2 + |\nabla \psi|^2 \right) \xi^2 \leq C \left(\int_{\mathbb{R}^3} R_m \psi \xi^2 + \int_{\mathbb{R}^3} (w^2 + \psi^2) |\nabla \xi|^2 \right). \quad (6.41)$$

To control the ψ -dependence on the right-hand side of (6.41), we require an estimate of the form

$$\int_{\mathbb{R}^3} \psi^2 \xi^2 \leq C \left(\int_{\mathbb{R}^3} R_m \psi \xi^2 + \int_{\mathbb{R}^3} (w^2 + \psi^2) |\nabla \xi|^2 \right), \quad (6.42)$$

which holds for $\xi \in H_1$, i.e. $\xi \in H^1(\mathbb{R}^3)$ satisfying $|\nabla \xi| \leq \xi$ on \mathbb{R}^3 .

Suppose (6.42) holds, then applying Hölder's inequality and (6.41) yields

$$\int_{\mathbb{R}^3} (w^2 + \psi^2) \xi^2 \leq C' \left(\int_{\mathbb{R}^3} R_m^2 \xi^2 + \int_{\mathbb{R}^3} (w^2 + \psi^2) |\nabla \xi|^2 \right).$$

To remove the term $\int (w^2 + \psi^2) |\nabla \xi|^2$ on the right-hand side, we simply restrict from $\xi \in H_1$ to a narrower class of test functions,

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

where $\gamma = \min\{1, (2C')^{-1/2}\} > 0$, to show

$$\int_{\mathbb{R}^3} \left(w^2 + |\nabla w|^2 + \psi^2 + |\nabla \psi|^2 \right) \xi^2 \leq 2C' \int_{\mathbb{R}^3} R_m^2 \xi^2. \quad (6.43)$$

In order to show (6.42), we adapt the argument used in [7]. At the same time, since the equations for (w, ψ) hold pointwise, we obtain additional estimates for $\Delta w, \Delta \psi$.

Lemma 6.4. *Suppose (A) holds, then there exists $C = C(M, M', \omega)$, $\gamma = \gamma(M, M', \omega) > 0$ such that for any $\xi \in H_\gamma$*

$$\int_{\mathbb{R}^3} \left(w^2 + |\nabla w|^2 + |\Delta w|^2 + \psi^2 + |\nabla \psi|^2 + |\Delta \psi|^2 \right) \xi^2 \leq C \int_{\mathbb{R}^3} R_m^2 \xi^2. \quad (6.44)$$

Clearly Lemmas 6.3 and 6.4 hold also under the assumption (B) since (B) implies (A), with $M' = C(M)$. In the case (B) where m_1, m_2 are both uniformly bounded below and have higher regularity, arguing as in Corollary 3.1 and Lemma 6.4, we obtain improved estimates for w and ψ .

Observe that in Case (B), $M' = C(M)$. Due to this, we omit the dependence of M' in the constants that appear in the following lemmas, whenever we assume (B) holds.

Lemma 6.5. *Suppose that either (A) or (B) holds, then there exist $C = C_A(M, M', \omega)$, $\gamma = \gamma_A(M, M', \omega) > 0$ or $C = C_B(k, M, \omega)$, $\gamma = \gamma_B(M, \omega) > 0$, where γ_B independent of k , such that for any $\xi \in H_\gamma$*

$$\int_{\mathbb{R}^3} \left(\sum_{|\alpha_1| \leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \leq k+2} |\partial^{\alpha_2} \psi|^2 \right) \xi^2 \leq C \int_{\mathbb{R}^3} \sum_{|\beta| \leq k} |\partial^\beta R_m|^2 \xi^2. \quad (6.45)$$

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

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(y)|^2 \leq C \int_{\mathbb{R}^3} \sum_{|\beta| \leq k} |\partial^\beta R_m(x)|^2 e^{-2\gamma|x-y|} dx. \quad (6.46)$$

We remark that in the following proofs, all integrals are taken over \mathbb{R}^3 , unless stated otherwise.

Proof (Proof of Lemma 6.3). *Case 1.* First suppose that $m_2 \neq 0$ and $u_2 > 0$. Recall that $m_1 \in \mathcal{M}_{L^2}(M, \omega)$, hence by Propositions 3.1, 3.2 and (6.40)

$$\begin{aligned} \|u_1\|_{H_{\text{unif}}^4(\mathbb{R}^3)} + \|\phi_1\|_{H_{\text{unif}}^2(\mathbb{R}^3)} &\leq C(M), \\ \|u_2\|_{H_{\text{unif}}^4(\mathbb{R}^3)} + \|\phi_2\|_{H_{\text{unif}}^2(\mathbb{R}^3)} &\leq C(M'), \\ \inf_{x \in \mathbb{R}^3} u_1(x) &\geq c_{M,\omega} > 0. \end{aligned}$$

By the Sobolev embedding: for all $k \in \mathbb{N}_0$ and $x \in \mathbb{R}^3$ $H^{k+2}(B_1(x)) \hookrightarrow C^{k,1/2}(B_1(x))$, so it follows that

$$\begin{aligned} \|u_1\|_{W^{2,\infty}(\mathbb{R}^3)} + \|\phi_1\|_{L^\infty(\mathbb{R}^3)} &\leq C(M), \\ \|u_2\|_{W^{2,\infty}(\mathbb{R}^3)} + \|\phi_2\|_{L^\infty(\mathbb{R}^3)} &\leq C(M'), \end{aligned}$$

hence $w = u_1 - u_2 \in H_{\text{unif}}^4(\mathbb{R}^3) \cap W^{2,\infty}(\mathbb{R}^3)$, $\psi = \phi_1 - \phi_2 \in H_{\text{unif}}^2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, and solve

$$-\Delta w = \frac{5}{3} \left(u_2^{7/3} - u_1^{7/3} \right) + \phi_1 u_1 - \phi_2 u_2, \quad (6.47a)$$

$$-\Delta \psi = 4\pi \left(u_2^2 - u_1^2 \right) + R_m, \quad (6.47b)$$

pointwise. Let $\xi \in H^1(\mathbb{R}^3)$ then test (6.47a) with $w\xi^2$ to obtain

$$\int \nabla w \cdot \nabla (w\xi^2) + \frac{5}{3} \int \left(u_1^{7/3} - u_2^{7/3} \right) w\xi^2 - \int (\phi_1 u_1 - \phi_2 u_2) w\xi^2 = 0. \quad (6.48)$$

We will use the following rearrangements

$$\phi_1 u_1 - \phi_2 u_2 = \frac{\phi_1 + \phi_2}{2} w + \frac{u_1 + u_2}{2} \psi, \quad (6.49)$$

$$\int \nabla w \cdot \nabla (w\xi^2) = \int |\nabla(w\xi)|^2 - \int w^2 |\nabla \xi|^2, \quad (6.50)$$

$$\int \nabla \psi \cdot \nabla (\psi\xi^2) = \int |\nabla(\psi\xi)|^2 - \int \psi^2 |\nabla \xi|^2. \quad (6.51)$$

To estimate the second term of (6.48), observe that Proposition 3.2 and (A) imply that $\inf u_1 \geq c_{M,\omega} > 0$ and recall the assumption $u_2 > 0$. It follows that for $v = \frac{1}{2} \inf(u_1^{4/3} + u_2^{4/3}) \geq \frac{1}{2} c_{M,\omega}^{4/3} > 0$

$$\begin{aligned} (u_1^{7/3} - u_2^{7/3})(u_1 - u_2) &= (u_1^{4/3} + u_2^{4/3})w^2 + u_1 u_2 (u_1^{1/3} - u_2^{1/3})w \\ &\geq (u_1^{4/3} + u_2^{4/3})w^2 \\ &\geq \frac{1}{2} (u_1^{4/3} + u_2^{4/3})w^2 + v w^2. \end{aligned} \quad (6.52)$$

Combining the estimates (6.48)–(6.50) and (6.52), we obtain

$$\begin{aligned} \int |\nabla(w\xi)|^2 + \frac{5}{6} \int (u_1^{4/3} + u_2^{4/3})w^2 \xi^2 - \frac{1}{2} \int (\phi_1 + \phi_2)w^2 \xi^2 + v \int w^2 \xi^2 \\ \leq \int w^2 |\nabla \xi|^2 + \frac{1}{2} \int \psi (u_1^2 - u_2^2) \xi^2. \end{aligned} \quad (6.53)$$

We define the following operators

$$\begin{aligned} L_1 &= -\Delta + \frac{5}{3}u_1^{4/3} - \phi_1, \\ L_2 &= -\Delta + \frac{5}{3}u_2^{4/3} - \phi_2, \\ L &= \frac{1}{2}L_1 + \frac{1}{2}L_2 = -\Delta + \frac{5}{6}(u_1^{4/3} + u_2^{4/3}) - \frac{1}{2}(\phi_1 + \phi_2). \end{aligned}$$

As $u_1, u_2 > 0$, Lemma 6.2 implies that L_1, L_2 are non-negative operators, hence for any $\varphi \in H^1(\mathbb{R}^3)$

$$\langle \varphi, L\varphi \rangle = \frac{1}{2} \langle \varphi, L_1\varphi \rangle + \frac{1}{2} \langle \varphi, L_2\varphi \rangle \geq 0. \quad (6.54)$$

Observe that as $w \in W^{2,\infty}(\mathbb{R}^3)$ and $\xi \in H^1(\mathbb{R}^3)$, $w\xi \in H^1(\mathbb{R}^3)$. We can express (6.53) as

$$\langle w\xi, L(w\xi) \rangle + v \int w^2 \xi^2 \leq \int w^2 |\nabla \xi|^2 + \frac{1}{2} \int \psi (u_1^2 - u_2^2) \xi^2. \quad (6.55)$$

To control the final term of (6.55), we begin by testing (6.47b) with $\psi \xi^2$ to obtain

$$\int \nabla \psi \cdot \nabla (\psi \xi^2) = 4\pi \int \psi (u_2^2 - u_1^2) \xi^2 + \int R_m \psi \xi^2. \quad (6.56)$$

Rearranging (6.56) and applying (6.51) yields

$$\begin{aligned} \frac{1}{2} \int \psi (u_1^2 - u_2^2) \xi^2 &= \frac{1}{8\pi} \int R_m \psi \xi^2 - \frac{1}{8\pi} \int \nabla \psi \cdot \nabla (\psi \xi^2) \\ &= \frac{1}{8\pi} \int R_m \psi \xi^2 - \frac{1}{8\pi} \int |\nabla(\psi \xi)|^2 + \frac{1}{8\pi} \int \psi^2 |\nabla \xi|^2. \end{aligned} \quad (6.57)$$

Combining (6.55) and (6.57) yields

$$\begin{aligned} \langle w\xi, L(w\xi) \rangle + \nu \int w^2 \xi^2 + \frac{1}{8\pi} \int |\nabla(\psi\xi)|^2 \\ \leq \frac{1}{8\pi} \int R_m \psi \xi^2 + \int w^2 |\nabla \xi|^2 + \frac{1}{8\pi} \int \psi^2 |\nabla \xi|^2. \end{aligned} \quad (6.58)$$

As $\xi \nabla \psi = \nabla(\psi\xi) - \psi \nabla \xi$, we have

$$\begin{aligned} \int |\nabla \psi|^2 \xi^2 &\leq C \left(\int |\nabla(\psi\xi)|^2 + \int \psi^2 |\nabla \xi|^2 \right) \\ &\leq C \left(\int R_m \psi \xi^2 + \int (w^2 + \psi^2) |\nabla \xi|^2 \right). \end{aligned} \quad (6.59)$$

Combining the estimates (6.58)–(6.59), we obtain

$$\begin{aligned} \langle w\xi, L(w\xi) \rangle + \nu \int w^2 \xi^2 + \int |\nabla \psi|^2 \xi^2 \\ \leq C \left(\int R_m \psi \xi^2 + \int (w^2 + \psi^2) |\nabla \xi|^2 \right). \end{aligned} \quad (6.60)$$

Next we obtain an estimate for $\int |\nabla w|^2 \xi^2$, using the fact that L is a non-negative operator. We can express L as

$$L = -\Delta + a, \quad \text{where } a = \frac{5(u_1^{4/3} + u_2^{4/3})}{6} - \frac{\phi_1 + \phi_2}{2} \in H_{\text{unif}}^2(\mathbb{R}^3).$$

From (6.54), we have shown that $L = -\Delta + a \geq 0$ in the sense that $\langle \varphi, L\varphi \rangle \geq 0$ for every $\varphi \in H^1(\mathbb{R}^3)$. So for $\varepsilon \in (0, 1)$

$$L = (1 - \varepsilon)(-\Delta + a) + \varepsilon(-\Delta) + \varepsilon a \geq \varepsilon(-\Delta) - \varepsilon \|a\|_{L^\infty(\mathbb{R}^3)}.$$

Applying this to (6.60) gives

$$\begin{aligned} \varepsilon \int |\nabla(w\xi)|^2 + (\nu - \varepsilon \|a\|_{L^\infty(\mathbb{R}^3)}) \int w^2 \xi^2 \\ \leq C \left(\int R_m \psi \xi^2 + \int (w^2 + \psi^2) |\nabla \xi|^2 \right), \end{aligned}$$

so choosing $\varepsilon = \min\{\frac{\nu}{2\|a\|_{L^\infty}}, \frac{1}{2}\}$, we deduce

$$\int |\nabla(w\xi)|^2 \leq C \left(\int R_m \psi \xi^2 + \int (w^2 + \psi^2) |\nabla \xi|^2 \right)$$

and since $\xi \nabla w = \nabla(w\xi) - w \nabla \xi$, we deduce

$$\int |\nabla w|^2 \xi^2 \leq C \left(\int R_m \psi \xi^2 + \int (w^2 + \psi^2) |\nabla \xi|^2 \right). \quad (6.61)$$

We combine the estimates (6.60) and (6.61) to obtain the desired estimate (6.41)

$$\int w^2 \xi^2 + \int |\nabla w|^2 \xi^2 + \int |\nabla \psi|^2 \xi^2 \leq C \left(\int R_m \psi \xi^2 + \int (w^2 + \psi^2) |\nabla \xi|^2 \right)$$

and observe that this estimate is valid for any $\xi \in H^1(\mathbb{R}^3)$.

Case 2. Suppose now that $m_2 = u_2 = \phi_2 = 0$, then the argument used to show (6.53) holds to give

$$\begin{aligned} & \int |\nabla(w\xi)|^2 + \frac{5}{6} \int u_1^{4/3} w^2 \xi^2 - \frac{1}{2} \int \phi_1 w^2 \xi^2 + \nu \int w^2 \xi^2 \\ & \leq \int w^2 |\nabla \xi|^2 + \frac{1}{2} \int \psi u_1^2 \xi^2. \end{aligned} \quad (6.62)$$

Now using that L_1 is a non-negative operator, we obtain

$$\begin{aligned} \frac{1}{2} \int |\nabla(w\xi)|^2 + \nu \int w^2 \xi^2 & \leq \frac{1}{2} \langle \varphi, L_1 \varphi \rangle + \frac{1}{2} \int |\nabla(w\xi)|^2 + \nu \int w^2 \xi^2 \\ & = \int |\nabla(w\xi)|^2 + \frac{5}{6} \int u_1^{4/3} w^2 \xi^2 - \frac{1}{2} \int \phi_1 w^2 \xi^2 + \nu \int w^2 \xi^2 \\ & \leq \int w^2 |\nabla \xi|^2 + \frac{1}{2} \int \psi u_1^2 \xi^2. \end{aligned}$$

Then applying the estimates (6.56)–(6.60) yields the desired estimate (6.41): for all $\xi \in H^1(\mathbb{R}^3)$

$$\int w^2 \xi^2 + \int |\nabla w|^2 \xi^2 + \int |\nabla \psi|^2 \xi^2 \leq C \left(\int R_m \psi \xi^2 + \int (w^2 + \psi^2) |\nabla \xi|^2 \right)$$

□

Proof (Proof of Lemma 6.4). To obtain an integral estimate for ψ , first recall (6.47a), that w solves

$$-\Delta w + \frac{5}{3} \left(u_1^{7/3} - u_2^{7/3} \right) - \frac{\phi_1 + \phi_2}{2} w = \frac{u_1 + u_2}{2} \psi,$$

then testing this equation with $\psi \xi^2$, for $\xi \in H^1(\mathbb{R}^3)$, yields

$$\int \frac{u_1 + u_2}{2} \psi^2 \xi^2 = - \int \Delta w \psi \xi^2 + \frac{5}{3} \int \left(u_1^{7/3} - u_2^{7/3} \right) \psi \xi^2 - \int \frac{\phi_1 + \phi_2}{2} w \psi \xi^2. \quad (6.63)$$

The first term of the right-hand side can be estimated using integration by parts

$$\begin{aligned} \left| \int \Delta w \psi \xi^2 \right| & = \left| \int \nabla w \cdot \nabla (\psi \xi^2) \right| \leq \left| \int \nabla w \cdot \nabla \psi \xi^2 \right| + 2 \left| \int \nabla w \cdot \nabla \xi \psi \xi \right| \\ & \leq \left(\int |\nabla w|^2 \xi^2 \right)^{1/2} \left(\int |\nabla \psi|^2 \xi^2 \right)^{1/2} + 2 \left(\int |\nabla w|^2 |\nabla \xi|^2 \right)^{1/2} \left(\int \psi^2 \xi^2 \right)^{1/2}. \end{aligned}$$

By restricting $\xi \in H_1$, we have $|\nabla \xi| \leq |\xi|$ hence

$$\left| \int \Delta w \psi \xi^2 \right| \leq 2 \left(\int |\nabla w|^2 \xi^2 \right)^{1/2} \left(\int \psi^2 \xi^2 \right)^{1/2} + \int (|\nabla w|^2 + |\nabla \psi|^2) \xi^2. \quad (6.64)$$

We now estimate the remaining terms on the right-hand side of (6.63)

$$\begin{aligned} & \left| \frac{5}{3} \int (u_1^{7/3} - u_2^{7/3}) \psi \xi^2 - \int \frac{\phi_1 + \phi_2}{2} w \psi \xi^2 \right| \\ & \leq C \int |w| |\psi| \xi^2 \leq C \left(\int w^2 \xi^2 \right)^{1/2} \left(\int \psi^2 \xi^2 \right)^{1/2}. \end{aligned} \quad (6.65)$$

Combining the estimates (6.64)–(6.65) with (6.63) and using that $\inf u_1 \geq c_{M,\omega} > 0$ and $u_2 \geq 0$, we obtain

$$\begin{aligned} \int \psi^2 \xi^2 & \leq \frac{2}{c_{M,\omega}} \int \frac{u_1 + u_2}{2} \psi^2 \xi^2 \leq C \left[\left(\int |\nabla w|^2 \xi^2 \right)^{1/2} + \left(\int w^2 \xi^2 \right)^{1/2} \right] \left(\int \psi^2 \xi^2 \right)^{1/2} \\ & \quad + \int (|\nabla w|^2 + |\nabla \psi|^2) \xi^2 \end{aligned} \quad (6.66)$$

Applying Young's inequality twice and using (6.41) of Lemma 6.3 yields

$$\begin{aligned} \int \psi^2 \xi^2 & \leq \frac{1}{2} \int \psi^2 \xi^2 + C \int (w^2 + |\nabla w|^2 + |\nabla \psi|^2) \xi^2 \\ & \leq \frac{1}{2} \int \psi^2 \xi^2 + C \left(\int R_m \psi \xi^2 + \int (w^2 + \psi^2) |\nabla \xi|^2 \right) \\ & \leq \frac{3}{4} \int \psi^2 \xi^2 + C \left(\int R_m^2 \xi^2 + \int (w^2 + \psi^2) |\nabla \xi|^2 \right), \end{aligned}$$

hence we obtain

$$\int (w^2 + |\nabla w|^2 + \psi^2 + |\nabla \psi|^2) \xi^2 \leq C \left(\int R_m^2 \xi^2 + \int (w^2 + \psi^2) |\nabla \xi|^2 \right). \quad (6.67)$$

We further restrict the choice of the test function ξ , to remove the terms depending on w and ψ from the right-hand side. Given $C = C(M', M, \omega) > 0$, define $\gamma = \min\{1, (2C)^{-1/2}\} > 0$. First note that $H_\gamma \subseteq H_1$, so for any $\xi \in H_\gamma$ the estimate (6.67) continues to hold. In addition, $|\nabla \xi| \leq \gamma |\xi|$, hence

$$\begin{aligned} & \int (w^2 + |\nabla w|^2 + \psi^2 + |\nabla \psi|^2) \xi^2 \\ & \leq C \left(\int R_m^2 \xi^2 + \int (w^2 + \psi^2) |\nabla \xi|^2 \right) \\ & \leq C \left(\int R_m^2 \xi^2 + \tilde{\gamma}^2 \int (w^2 + \psi^2) \xi^2 \right) \leq C \int R_m^2 \xi^2 + \frac{1}{2} \int (w^2 + \psi^2) \xi^2. \end{aligned}$$

After re-arranging, it follows that for any $\xi \in H_\gamma$

$$\int \left(w^2 + |\nabla w|^2 + \psi^2 + |\nabla \psi|^2 \right) \xi^2 \leq C \int R_m^2 \xi^2. \quad (6.68)$$

Finally, as the equations (6.47) hold pointwise, squaring each equation and integrating them against ξ^2 yields

$$\begin{aligned} \int |\Delta w|^2 \xi^2 &\leq C \int \left(w^2 + \psi^2 \right) \xi^2 \\ \int |\Delta \psi|^2 \xi^2 &\leq C \int \left(R_m^2 + w^2 \right) \xi^2. \end{aligned}$$

Combining these estimates with (6.67), we obtain the desired result (6.44)

$$\int \left(w^2 + |\nabla w|^2 + |\Delta w|^2 + \psi^2 + |\nabla \psi|^2 + |\Delta \psi|^2 \right) \xi^2 \leq C \int R_m^2 \xi^2.$$

□

Proof (Proof of Lemma 6.5). *Case 1.* Suppose (B) holds, so $m_i \in \mathcal{M}_{H^k}(M, \omega)$ for some $k \in \mathbb{N}_0$. By Corollary 3.1, for $i \in \{1, 2\}$

$$\|u_i\|_{H_{\text{unif}}^{k+4}(\mathbb{R}^3)} + \|\phi_i\|_{H_{\text{unif}}^{k+2}(\mathbb{R}^3)} \leq C(k, M, \omega). \quad (6.69)$$

Using integration by parts, we shall obtain integral estimates for derivatives of w in terms of derivatives of Δw . We will use the Einstein summation convention throughout this proof.

To begin, we approximate $w \in H_{\text{unif}}^{k+4}(\mathbb{R}^3)$ by smooth functions $w_h \in C^\infty(\mathbb{R}^3)$ such that for all $|\beta| \leq k+4$, $\partial^\beta w_h$ converges to $\partial^\beta w$ pointwise [26]. This approximation is necessary in order to obtain estimates for $\partial^\alpha w$ when $|\alpha| = k+4$.

Fix $\xi \in H_\gamma$ and let $|\beta| = k' \leq k+2$. Then using integration by parts gives

$$\begin{aligned} \int \left| \Delta \partial^\beta w_h \right|^2 \xi^2 &= \int \partial_{ii} \partial^\beta w_h \partial_{jj} \partial^\beta w_h \xi^2 \\ &= - \int \partial_i \partial^\beta w_h \partial_{ijj} \partial^\beta w_h \xi^2 - 2 \int \partial_i \partial^\beta w_h \partial_{jj} \partial^\beta w_h \xi \partial_i \xi \\ &= \int \partial_{ij} \partial^\beta w_h \partial_{ij} \partial^\beta w_h \xi^2 + 2 \int \partial_i \partial^\beta w_h \partial_{ij} \partial^\beta w_h \xi \partial_j \xi - 2 \int \partial_i \partial^\beta w_h \partial_{jj} w_h \xi \partial_i \xi \\ &= \int \sum_{|\alpha|=2} \left| \partial^{\alpha+\beta} w \right|^2 \xi^2 + 2 \int \partial_i \partial^\beta w_h \partial_{ij} \partial^\beta w_h \xi \partial_j \xi - 2 \int \partial_i \partial^\beta w_h \partial_{jj} \partial^\beta w_h \xi \partial_i \xi. \end{aligned}$$

Summing over $|\beta| = k'$ and rearranging yields

$$\begin{aligned} \int \sum_{|\alpha|=k'+2} \left| \partial^\alpha w_h \right|^2 \xi^2 &= \int \sum_{|\beta|=k'} \left| \Delta \partial^\beta w_h \right|^2 \xi^2 \\ &\quad + 2 \sum_{|\beta|=k'} \sum_{i,j=1}^3 \left(\int \partial_i \partial^\beta w_h \partial_{ij} \partial^\beta w_h \xi \partial_j \xi - \int \partial_i \partial^\beta w_h \partial_{jj} \partial^\beta w_h \xi \partial_i \xi \right). \end{aligned}$$

Then, using that $\xi \in H_\gamma \subseteq H_1$, hence $|\nabla \xi| \leq |\xi|$, we can estimate the right-hand side using Hölder's inequality,

$$\begin{aligned} \int \sum_{|\alpha|=k'+2} |\partial^\alpha w_h|^2 \xi^2 &\leq \int \sum_{|\beta|=k'} |\Delta \partial^\beta w_h|^2 \xi^2 \\ &\quad + C \sum_{|\beta|=k'} \sum_{i,j=1}^3 \left(\int |\partial_i \partial^\beta w_h| |\partial_{ij} \partial^\beta w_h| \xi^2 + \int |\partial_i \partial^\beta w_h| |\partial_{jj} \partial^\beta w_h| \xi^2 \right) \\ &\leq \frac{1}{2} \int \sum_{|\alpha|=k'+2} |\partial^\alpha w_h|^2 \xi^2 + C \left(\int \sum_{|\beta_1|=k'} |\Delta \partial^{\beta_1} w_h|^2 \xi^2 + \int \sum_{|\beta_2|=k'+1} |\partial^{\beta_2} w_h|^2 \xi^2 \right). \end{aligned}$$

Re-arranging this and letting $h \rightarrow 0$, we obtain

$$\sum_{|\alpha|=k'+2} \int |\partial^\alpha w|^2 \xi^2 \leq C \left(\int \sum_{|\beta_1|=k'} |\partial^{\beta_1} \Delta w|^2 \xi^2 + \int \sum_{|\beta_2|=k'+1} |\partial^{\beta_2} w|^2 \xi^2 \right). \quad (6.70)$$

Using an identical argument, we obtain similar estimates for ψ , for $k' \leq k$,

$$\sum_{|\alpha|=k'+2} \int |\partial^\alpha \psi|^2 \xi^2 \leq C \left(\int \sum_{|\beta_1|=k'} |\partial^{\beta_1} \Delta \psi|^2 \xi^2 + \int \sum_{|\beta_2|=k'+1} |\partial^{\beta_2} \psi|^2 \xi^2 \right). \quad (6.71)$$

In the case $k' = 0$, combining (6.70), (6.71) and (6.44) of Lemma 6.4 yields: there exists $C, \gamma > 0$ such that for all $\xi \in H_\gamma$

$$\begin{aligned} \int \sum_{|\alpha|=2} (|\partial^\alpha w|^2 + |\partial^\alpha \psi|^2) \xi^2 \\ \leq C \int (|\nabla w|^2 + |\Delta w|^2 + |\nabla \psi|^2 + |\Delta \psi|^2) \xi^2 \leq C \int R_m^2 \xi^2. \end{aligned} \quad (6.72)$$

We will now provide estimates for the right-hand terms of the form $\partial^\beta \Delta w$, $\partial^\beta \Delta \psi$. Recall (6.47)

$$\begin{aligned} -\Delta w &= \frac{5}{3} (u_2^{7/3} - u_1^{7/3}) + \frac{\phi_1 + \phi_2}{2} w + \frac{u_1 + u_2}{2} \psi =: f_1, \\ -\Delta \psi &= 4\pi (u_2^2 - u_1^2) + R_m =: f_2. \end{aligned}$$

From (6.69) it follows that $f_1 \in H_{\text{unif}}^{k+2}(\mathbb{R}^3)$, $f_2 \in H_{\text{unif}}^k(\mathbb{R}^3)$. Let $|\alpha_1| = j_1 \leq k+2$, $|\alpha_2| = j_2 \leq k$, then differentiating (6.47) yields

$$|\partial^{\alpha_1} \Delta w| \leq C(j_1, M, \omega) \sum_{|\beta_1| \leq j_1} (|\partial^{\beta_1} w| + |\partial^{\beta_1} \psi|), \quad (6.73)$$

$$|\partial^{\alpha_2} \Delta \psi| \leq C(j_2, M, \omega) \sum_{|\beta_2| \leq j_2} (|\partial^{\beta_2} R_m| + |\partial^{\beta_2} w|). \quad (6.74)$$

Squaring (6.73)–(6.74), summing over partial derivatives and integrating against ξ^2 we deduce

$$\int \sum_{|\alpha_1|=j_1} |\partial^{\alpha_1} \Delta w|^2 \xi^2 \leq C \int \sum_{|\beta_1| \leq j_1} \left(|\partial^{\beta_1} w|^2 + |\partial^{\beta_1} \psi|^2 \right) \xi^2, \quad (6.75)$$

$$\int \sum_{|\alpha_2|=j_2} |\partial^{\alpha_2} \Delta \psi|^2 \xi^2 \leq C \int \sum_{|\beta_2| \leq j_2} \left(|\partial^{\beta_2} R_m|^2 + |\partial^{\beta_2} w|^2 \right) \xi^2. \quad (6.76)$$

Substituting (6.75) into (6.70) gives for $i \leq k+4$

$$\begin{aligned} \int \sum_{|\alpha|=i_1} |\partial^\alpha w|^2 \xi^2 &\leq C \int \left(\sum_{|\beta_1|=i_1-1} |\partial^{\beta_1} w|^2 + \sum_{|\beta_2|=i_1-2} |\partial^{\beta_2} \Delta w|^2 \right) \xi^2 \\ &\leq C \int \left(\sum_{|\beta_1|=i_1-1} |\partial^{\beta_1} w|^2 + \sum_{|\beta_1| \leq i_1-2} \left(|\partial^{\beta_1} w|^2 + |\partial^{\beta_1} \psi|^2 \right) \right) \xi^2. \end{aligned} \quad (6.77)$$

Similarly, substituting (6.76) into (6.71) gives for $i_2 \leq k+2$

$$\begin{aligned} \int \sum_{|\alpha|=i_2} |\partial^\alpha \psi|^2 \xi^2 &\leq C \int \left(\sum_{|\beta_1|=i_2-1} |\partial^{\beta_1} \psi|^2 + \sum_{|\beta_2|=i_2-2} |\partial^{\beta_2} \Delta \psi|^2 \right) \xi^2 \\ &\leq C \int \left(\sum_{|\beta_1|=i_2-1} |\partial^{\beta_1} \psi|^2 + \sum_{|\beta_2| \leq i_2-2} \left(|\partial^{\beta_2} R_m|^2 + |\partial^{\beta_2} w|^2 \right) \right) \xi^2. \end{aligned} \quad (6.78)$$

Using (6.77) and (6.78), arguing by induction over i_1, i_2 simultaneously gives

$$\int \sum_{|\alpha| \leq k+2} \left(|\partial^\alpha w|^2 + |\partial^\alpha \psi|^2 \right) \xi^2 \leq C \int \sum_{|\beta| \leq k} |\partial^\beta R_m|^2 \xi^2.$$

To show the remaining estimate for the derivatives of w , applying (6.77) with $i_1 = k+3, k+4$ yields the estimate (6.45)

$$\int \left(\sum_{|\alpha_1| \leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \leq k+2} |\partial^{\alpha_2} \psi|^2 \right) \xi^2 \leq C \int \sum_{|\beta| \leq k} |\partial^\beta R_m|^2 \xi^2.$$

Now fix $y \in \mathbb{R}^3$ and choose $\xi(x) = e^{-\gamma|x-y|}$. We will now show the lower pointwise lower bound for w and ψ

$$\begin{aligned} &\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(y)|^2 \\ &\leq C \int \left(\sum_{|\alpha_1| \leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \leq k+2} |\partial^{\alpha_2} \psi|^2 \right) e^{-2\gamma|x-y|} dx, \end{aligned} \quad (6.79)$$

where the constant C is independent of y and γ .

By Corollary 3.1, $w \in H^{k+4}(B_1(y))$, $\psi \in H^{k+2}(B_1(y))$, hence by the Sobolev embedding theorem [20] $w \in C^{k+2,1/2}(B_1(y))$, $\psi \in C^{k,1/2}(B_1(y))$ and

$$\begin{aligned}\|w\|_{C^{k+2}(B_1(y))} &\leq C \|w\|_{H^{k+4}(B_1(y))}, \\ \|\psi\|_{C^k(B_1(y))} &\leq C \|\psi\|_{H^{k+2}(B_1(y))}.\end{aligned}$$

We use these estimates to show (6.79)

$$\begin{aligned}&\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(y)|^2 \\&\leq \|w\|_{C^{k+2,1/2}(B_1(y))}^2 + \|\psi\|_{C^{k,1/2}(B_1(y))}^2 \\&\leq C \left(\|w\|_{H^{k+4}(B_1(y))}^2 + \|\psi\|_{H^{k+2}(B_1(y))}^2 \right) \\&= C \int_{B_1(y)} \left(\sum_{|\alpha_1| \leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \leq k+2} |\partial^{\alpha_2} \psi|^2 \right) \\&\leq C \int_{\mathbb{R}^3} \left(\sum_{|\alpha_1| \leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \leq k+2} |\partial^{\alpha_2} \psi|^2 \right) e^{-2\gamma|x-y|} dx.\end{aligned}$$

Combining (6.45) and (6.79), we obtain the desired estimate (6.46)

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(y)|^2 \leq C \int \sum_{|\beta| \leq k} |\partial^\beta R_m(x)|^2 e^{-2\gamma|x-y|} dx.$$

Case 2. Suppose (A) holds, then as $m_1 \in \mathcal{M}_{L^2}(M, \omega)$, by Proposition 3.1 and (6.40),

$$\begin{aligned}\|u_1\|_{H_{\text{unif}}^4(\mathbb{R}^3)} + \|\phi_1\|_{H_{\text{unif}}^2(\mathbb{R}^3)} &\leq C(M), \\ \|u_2\|_{H_{\text{unif}}^4(\mathbb{R}^3)} + \|\phi_2\|_{H_{\text{unif}}^2(\mathbb{R}^3)} &\leq C(M').\end{aligned}$$

The argument used to show (6.70) holds for $k' \leq 2$, so for $\xi \in H_1$

$$\sum_{|\alpha_1| \leq 4} \int |\partial^{\alpha_1} w|^2 \xi^2 \leq C \left(\int \sum_{|\beta_1| \leq 2} |\partial^{\beta_1} \Delta w|^2 \xi^2 + \int \sum_{|\beta_2| \leq 2} |\partial^{\beta_2} w|^2 \xi^2 \right).$$

Then, as (6.75) holds with $j_1 \leq 2$, applying this and (6.70) for $k' = 0$ yields

$$\begin{aligned}\sum_{|\alpha_1| \leq 4} \int |\partial^{\alpha_1} w|^2 \xi^2 &\leq C \int \sum_{|\beta_1| \leq 2} \left(|\partial^{\beta_1} w|^2 + |\partial^{\beta_1} \psi|^2 \right) \xi^2 \\&\leq C \left(\int |\Delta w|^2 \xi^2 + \int \sum_{|\beta_1| \leq 1} |\partial^{\beta_1} w|^2 \xi^2 + \sum_{|\beta_2| \leq 2} |\partial^{\beta_2} w|^2 \xi^2 \right).\end{aligned}\tag{6.80}$$

Similarly, the argument used to show (6.71) holds for $k' = 0$, to give

$$\sum_{|\alpha_2| \leq 2} \int |\partial^{\alpha_2} \psi|^2 \xi^2 \leq C \left(\int |\Delta \psi|^2 \xi^2 + \int \sum_{|\beta_2| \leq 1} |\partial^{\beta_2} \psi|^2 \xi^2 \right). \quad (6.81)$$

Finally, combining (6.80)–(6.81) and applying (6.44) from Lemma 6.4, we obtain the desired estimate (6.45) with $k = 0$

$$\begin{aligned} & \sum_{|\alpha_1| \leq 4} \int |\partial^{\alpha_1} w|^2 \xi^2 + \sum_{|\alpha_2| \leq 2} \int |\partial^{\alpha_2} \psi|^2 \xi^2 \\ & \leq C \left(\int (|\Delta w|^2 + |\Delta \psi|^2) \xi^2 + \int \sum_{|\beta_1| \leq 1} \left(|\partial^{\beta_1} w|^2 + |\partial^{\beta_1} \psi|^2 \right) \xi^2 \right) \\ & \leq C \int R_m^2 \xi^2. \end{aligned}$$

The argument used in Case 1 holds for $k = 0$ to show the desired estimate (6.46)

$$\sum_{|\alpha_1| \leq 2} |\partial^{\alpha_1} w(y)|^2 + |\psi(y)|^2 \leq C \int |R_m(x)|^2 e^{-2\gamma|x-y|} dx.$$

□

We have now established all technical prerequisites to prove Theorems 3.1 and 3.2.

Proof (Proof of Theorem 3.2). Applying Lemmas 6.3–6.5 with the assumption (B) yields the desired estimates (3.10)–(3.11). □

Proof (Proof of Theorem 3.1). *Case 1.* Suppose $\text{spt}(m_2)$ is bounded and $m_2 \not\equiv 0$. We show assumption (A) is satisfied, so by applying Lemmas 6.3–6.5 we obtain the desired estimates (3.8)–(3.9).

Since $m_2 \in L^2_{\text{unif}}(\mathbb{R}^3)$, 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 $\int m_2 > 0$. Then, define the minimisation problem

$$I^{\text{TFW}}(m_2) = \inf \left\{ E^{\text{TFW}}(v, m_2) \mid v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_2 > 0 \right\},$$

which yields a unique solution (u_2, ϕ_2) to (2.4), satisfying $u_2 > 0$, using [31, Theorem 7.19]. Applying Proposition 3.1, we obtain the uniform estimates

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

Case 2. Suppose $m_2 = u_2 = \phi_2 = 0$, then by definition (u_2, ϕ_2) solve (2.6) and (A) is satisfied, so Lemmas 6.3–6.5 imply (3.8)–(3.9).

Case 3. Suppose $\text{spt}(m_2)$ is unbounded. By Proposition 6.1, there exists (u_2, ϕ_2) solving (2.6) corresponding to m_2 and satisfying $u_2 \geq 0$. As we can not guarantee that $u_2 > 0$, we can not apply Lemmas 6.3–6.5 directly to compare (u_1, ϕ_1) with (u_2, ϕ_2) . Instead we follow the proof of Proposition 6.1 and use a thermodynamic

limit argument to construct a sequence of functions $(u_{2,R_n}, \phi_{2,R_n})$ that satisfy (A) for sufficiently large R_n , which converges to (u_2, ϕ_2) .

Let $R_n \uparrow \infty$ and define $m_{2,R_n} := m_2 \cdot \chi_{B_{R_n}(0)}$, then as $m_2 \in L^2_{\text{unif}}(\mathbb{R}^3)$, $m_2 \geq 0$ 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 6.1, the minimisation problem

$$I^{\text{TFW}}(m_{2,R_n}) = \inf \left\{ E^{\text{TFW}}(v, m_{2,R_n}) \mid v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_{2,R_n} \right\},$$

defines a unique solution $(u_{2,R_n}, \phi_{2,R_n})$ to (2.4), satisfying $u_{2,R_n} > 0$ and

$$\|u_{2,R_n}\|_{H^4_{\text{unif}}(\mathbb{R}^3)} + \|\phi_{2,R_n}\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \leq C(M'), \quad (6.82)$$

where the constant is independent of R_n . Passing to the limit in (6.82), there exist $u_2 \in H^4_{\text{unif}}(\mathbb{R}^3)$, $\phi_2 \in H^2_{\text{unif}}(\mathbb{R}^3)$ such that, respectively, along a subsequence u_{2,R_n}, ϕ_{2,R_n} converges to u_2, ϕ_2 , 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 $|\alpha| \leq 2$, $\partial^\alpha u_{2,R_n}, \phi_{2,R_n}$ converges to $\partial^\alpha u_2, \phi_2$ pointwise. It follows that (u_2, ϕ_2) is a solution of (2.6) corresponding to m_2 , satisfying $u_2 \geq 0$ and (3.7)

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

In addition, $(u'_1, \phi'_1) = (u_1, \phi_1)$ and $(u'_2, \phi'_2) = (u_{2,R_n}, \phi_{2,R_n})$ satisfy assumption (A) for large R_n , so by Lemmas 6.3–6.5 that there exist $C, \gamma > 0$, independent of R_n , such that for large R_n and any $\xi \in H_\gamma$

$$\begin{aligned} & \int_{\mathbb{R}^3} \left(\sum_{|\alpha_1| \leq 4} |\partial^{\alpha_1}(u_1 - u_{2,R_n})|^2 + \sum_{|\alpha_2| \leq 2} |\partial^{\alpha_2}(\phi_1 - \phi_{2,R_n})|^2 \right) \xi^2 \\ & \leq C \int_{\mathbb{R}^3} (m_1 - m_{2,R_n})^2 \xi^2, \end{aligned} \quad (6.83)$$

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

$$\begin{aligned} & \sum_{|\alpha_1| \leq 2} |\partial^{\alpha_1}(u_1 - u_{2,R_n})(y)|^2 + |(\phi_1 - \phi_{2,R_n})(y)|^2 \\ & \leq C \int_{\mathbb{R}^3} |(m_1 - m_{2,R_n})(x)|^2 e^{-2\gamma|x-y|} dx. \end{aligned} \quad (6.84)$$

Using the pointwise convergence of $(u_{2,R_n}, \phi_{2,R_n})$ to (u_2, ϕ_2) , applying the Dominated Convergence Theorem and sending $R_n \rightarrow \infty$ in (6.83)–(6.84) we obtain the desired estimates (3.8)–(3.9). \square

6.3. Proofs of Applications

The proof of Proposition 4.1 is an application of Theorem 3.1.

Proof (Proof of Proposition 4.1). Observe that $(u_1, \phi_1) = (u, \phi)$ and $(u_2, \phi_2) = (u_\Omega, \phi_\Omega)$ satisfy the conditions of Theorem 3.1, there exist $C, \tilde{\gamma} > 0$, independent of Ω , such that for all $y \in \mathbb{R}^3$

$$\sum_{|\alpha| \leq 2} |\partial^\alpha (u - u_\Omega)(y)|^2 + |(\phi - \phi_\Omega)(y)|^2 \leq C \int_{\mathbb{R}^3} |(m - m_\Omega)(x)|^2 e^{-2\gamma|x-y|} dx.$$

Now let $y \in \Omega$, $d = \text{dist}(y, \partial\Omega)$ and observe that $m - m_\Omega \in L^2_{\text{unif}}(\mathbb{R}^3)$. Since $\sup_{x \in A} e^{-2\tilde{\gamma}|x|} \leq C \inf_{x \in A} e^{-2\tilde{\gamma}|x|}$ for any $A \subset B_1(z)$, $z \in \mathbb{R}^3$, with $C = C(\tilde{\gamma})$ independent of z , we have the bound

$$\int_{B_d(y)^c} |(m - m_\Omega)(x)|^2 e^{-2\tilde{\gamma}|x-y|} dx \leq C \left(\|m\|_{L^2_{\text{unif}}(\mathbb{R}^3)}^2 + \|m_\Omega\|_{L^2_{\text{unif}}(\mathbb{R}^3)}^2 \right) \int_{B_d(y)^c} e^{-2\tilde{\gamma}|x-y|} dx.$$

Therefore, we obtain the desired estimate (4.1)

$$\begin{aligned} \int_{\mathbb{R}^3} |(m - m_\Omega)(x)|^2 e^{-2\gamma|x-y|} dx &= \int_{\Omega^c} |(m - m_\Omega)(x)|^2 e^{-2\gamma|x-y|} dx \\ &\leq \int_{\Omega_{\text{buf}}^c} m(x)^2 e^{-2\tilde{\gamma}|x-y|} dx \leq CM^2 \int_{B_{R_{\text{buf}}}(0)^c} e^{-2\tilde{\gamma}|x-y|} dx \\ &\leq CM^2 \int_{B_d(y)^c} e^{-2\tilde{\gamma}|x-y|} dx \\ &= CM^2(1 + d^2)e^{-2\tilde{\gamma}d} \leq CM^2 e^{-2\gamma d}, \end{aligned}$$

for any given $0 < \gamma < \tilde{\gamma}$, where $C = C(\tilde{\gamma}, \gamma)$. \square

Next, we now prove Corollary 4.1 as a direct consequence of Theorems 3.1 and 3.2.

Proof (Proof of Corollary 4.1). Let $k \in \mathbb{N}_0$ and $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$ and recall the estimate (3.11) of Theorem 3.2, that there exists $C, \tilde{\gamma} > 0$ such that

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(y)|^2 \leq C \int \sum_{|\beta| \leq k} |\partial^\beta R_m(x)|^2 e^{-2\tilde{\gamma}|x-y|} dx. \quad (6.85)$$

(1) R_m having compact support is a special case of exponential decay, hence we consider only the case $\sum_{|\beta| \leq k} |\partial^\beta R_m(x)|^2 \leq C e^{-2\gamma'|x-z|}$. It is straightforward to see that there exists $C, \gamma > 0$, depending on $\tilde{\gamma}, \gamma'$, such that

$$\int_{\mathbb{R}^3} e^{-2\gamma'|x-z|} e^{-2\tilde{\gamma}|x-y|} dx \leq C e^{-2\gamma|y-z|}. \quad (6.86)$$

Hence (4.3) follows immediately from combining (6.85) and (6.86).

(2) Suppose that R_m satisfies the algebraic decay $\sum_{|\beta| \leq k} |\partial^\beta R_m(x)|^2 \leq C(1 + |x|)^{-2r}$. It is again elementary to show that there exists $C = C(r) > 0$ such that for all $y \in \mathbb{R}^3$

$$\int_{\mathbb{R}^3} (1 + |x|)^{-2r} e^{-2\gamma|x-y|} dx \leq C(1 + |y|)^{-2r}. \quad (6.87)$$

Combining (6.87) with (6.85) gives the desired estimate (4.4).

(3) Now suppose that $R_m \in H^k(\mathbb{R}^3)$ and recall (3.10) of Theorem 3.2, that there exists $C, \tilde{\gamma} > 0$ such that for all $\xi \in H_{\tilde{\gamma}}$

$$\int_{\mathbb{R}^3} \left(\sum_{|\alpha_1| \leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \leq k+2} |\partial^{\alpha_2} \psi|^2 \right) \xi^2 \leq C \int_{\mathbb{R}^3} \sum_{|\beta| \leq k} |\partial^\beta R_m|^2 \xi^2. \quad (6.88)$$

For any $0 < \gamma \leq \tilde{\gamma}$, the function $\xi_\gamma(x) = e^{-\gamma|x|} \in H_{\tilde{\gamma}}$. Then substituting ξ_γ into (6.88) yields

$$\begin{aligned} \int_{\mathbb{R}^3} \left(\sum_{|\alpha_1| \leq k+4} |\partial^{\alpha_1} w(x)|^2 + \sum_{|\alpha_2| \leq k+2} |\partial^{\alpha_2} \psi(x)|^2 \right) e^{-2\gamma|x|} dx \\ \leq C \int_{\mathbb{R}^3} \sum_{|\beta| \leq k} |\partial^\beta R_m(x)|^2 e^{-2\gamma|x|} dx \leq C \int_{\mathbb{R}^3} \sum_{|\beta| \leq k} |\partial^\beta R_m(x)|^2 dx. \end{aligned}$$

Sending $\gamma \rightarrow 0$ and applying the Dominated Convergence Theorem yields the desired estimate (4.5).

Under the assumptions of Theorem 3.1 with $k = 0$, other than applying Theorem 3.1 instead of Theorem 3.2, the proof is identical. \square

We turn to the proofs of the charge-neutrality estimates.

Proof (Proof of Theorem 4.1). Recall that $\rho_{12} = m_1 - u_1^2 - m_2 + u_2^2$. Let $R > 0$ and choose $\varphi_R \in C_c^\infty(\mathbb{R}^3)$ satisfying $0 \leq \varphi_R \leq 1$, $\varphi_R = 1$ on $B_R(0)$, $\varphi_R = 0$ outside $B_{R+1}(0)$ and $\|\varphi_R\|_{W^{2,\infty}(\mathbb{R}^3)} \leq c_\varphi$. Let $A_R := B_{R+1}(0) \setminus B_R(0)$. Recall (6.47b), that the difference $\psi := \phi_1 - \phi_2$ solves

$$-\Delta \psi = 4\pi \rho_{12} \quad (6.89)$$

pointwise. Testing (6.89) with φ_R and using integration by parts yields

$$\int_{B_{R+1}(0)} \rho_{12} \varphi_R = -\frac{1}{4\pi} \int_{A_R} \psi \Delta \varphi_R.$$

Since $\varphi_R = 1$ on $B_R(0)$, we deduce

$$\int_{B_R(0)} \rho_{12} = -\frac{1}{4\pi} \int_{A_R} \psi \Delta \varphi_R - \int_{A_R} \rho_{12} \varphi_R,$$

and hence

$$\left| \int_{B_R(0)} \rho_{12} \right| \leq C \int_{A_R} (|m_1 - m_2| + |u_1 - u_2| + |\phi_1 - \phi_2|), \quad (6.90)$$

where C depends only on c_φ . Observe that $|A_R| \leq CR^2$.

(1) By (4.3) of Corollary 4.1 there exists $C, \tilde{\gamma} > 0$ such that

$$|(\phi_1 - \phi_2)(x)| + |(m_1 - m_2)(x)| + |(u_1 - u_2)(x)| \leq C e^{-\tilde{\gamma}|x|}.$$

Then using (6.90) we deduce

$$\begin{aligned} \left| \int_{B_R(0)} \rho_{12} \right| &\leq C \int_{A_R} (|m_1 - m_2| + |u_1 - u_2| + |\phi_1 - \phi_2|) \\ &\leq C \int_{A_R} e^{-\tilde{\gamma}|x|} dx \leq C(1 + R^2)e^{-\tilde{\gamma}R}, \end{aligned} \quad (6.91)$$

which implies (4.9) for any $0 < \gamma < \tilde{\gamma}$.

(2) Suppose now that $|(m_1 - m_2)(x)| \leq C(1 + |x|)^{-r}$, then using (6.90) we obtain

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

(3) Suppose $m_1 - m_2 \in L^2(\mathbb{R}^3)$, then by Corollary 4.1, $u_1 - u_2, \phi_1 - \phi_2 \in H^2(\mathbb{R}^3)$, hence by Proposition 3.1 $u_1^2 - u_2^2 \in L^2(\mathbb{R}^3)$. Taking the Fourier transform, $\widehat{f}(k) = \int_{\mathbb{R}^3} f(x) e^{-2\pi i k \cdot x} dx$, of (6.89) and rearranging, we obtain

$$\frac{\widehat{\rho}_{12}(k)}{|k|^2} = \pi \widehat{\psi}(k) \in L^2(\mathbb{R}^3).$$

Arguing as in [10] we show that 0 is a Lebesgue point for $\widehat{\rho}_{12}$. For $\varepsilon > 0$,

$$\begin{aligned} \frac{1}{|B_\varepsilon(0)|} \int_{B_\varepsilon(0)} |\widehat{\rho}_{12}(k)| dk &\leq \frac{1}{|B_\varepsilon(0)|} \left(\int_{B_\varepsilon(0)} |k|^4 dk \right)^{1/2} \left(\int_{B_\varepsilon(0)} \frac{|\widehat{\rho}_{12}(k)|^2}{|k|^4} dk \right)^{1/2} \\ &\leq C \varepsilon^{1/2} \|\phi_1 - \phi_2\|_{L^2(\mathbb{R}^3)}, \end{aligned}$$

which tends to 0 as $\varepsilon \rightarrow 0$, as claimed. \square

6.4. Proof of Energy Locality

To prove Theorem 4.2, we first establish the existence, uniqueness and regularity of the solutions to the linearised TFW 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 $V \in \mathbb{R}^3 \setminus \{0\}$, $k \in \mathbb{N}$ and for $h \in [0, 1]$ define

$$Y^h = \{Y_j + \delta_{jk} h V \mid j \in \mathbb{N}\}, \quad (6.92)$$

and the associated nuclear configuration

$$m_h(x) = m(x) + \eta(x - Y_k - hV) - \eta(x - Y_k). \quad (6.93)$$

Lemma 6.6. *There exist $M', \omega'_0, \omega'_1 > 0$, such that for $\omega' = (\omega'_0, \omega'_1)$, $m_h \in \mathcal{M}_{L^2}(M', \omega')$ for all $h \in [0, 1]$. In particular, $Y^h \in \mathcal{Y}_{L^2}(M', \omega')$ for all $h \in [0, 1]$.*

Proof (Proof of Lemma 6.6). Recall that $m_h, \eta \geq 0, \eta \in C^\infty(\mathbb{R}^3)$ and $\int_{\mathbb{R}^3} \eta = 1$, then

$$\begin{aligned} \sup_{x \in \mathbb{R}^3} \|m_h\|_{L^2(B_1(x))} &\leq \sup_{x \in \mathbb{R}^3} \left(\|m\|_{L^2(B_1(x))} + \left(\int_{B_1(x)} \eta(z - Y_k - hV)^2 dz \right)^{1/2} \right) \\ &\leq M + \|\eta\|_{L^2(\mathbb{R}^3)} =: M'. \end{aligned}$$

Since $m \in \mathcal{M}_{L^2}(M, \omega)$, with $\omega = (\omega_0, \omega_1)$, for all $R > 0$,

$$\begin{aligned} \inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m_h(z) dz &\geq \inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m(z) dz - \int_{B_R(x)} \eta(z - Y_k) dz \\ &\geq \omega_0 R^3 - \omega_1 - 1, \end{aligned}$$

hence for $\omega' = (\omega_0, \omega_1 + 1)$, $m_h \in \mathcal{M}_{L^2}(M', \omega')$ for all $h \in [0, 1]$, as claimed. \square

As $m_h \in \mathcal{M}_{L^2}(M', \omega')$ for all $h \in [0, 1]$, by Theorem 2.1 there exists a corresponding ground state (u_h, ϕ_h) . Also, let $(u, \phi) = (u_0, \phi_0)$. We now use Corollary 4.1 to compare (u_h, ϕ_h) with (u, ϕ) and rigorously linearise the TFW equations.

Lemma 6.7. *Let $Y \in \mathcal{Y}_{L^2}(M, \omega)$ and let $m = m_Y \in \mathcal{M}_{L^2}(M, \omega)$. Also, let $k \in \mathbb{N}$, $V \in \mathbb{R}^3 \setminus \{0\}$ and $h_0 = \min\{1, |V|^{-1}\}$. For $h \in [0, h_0]$ define*

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

There exist $C = C(M', \omega')$, $\gamma_0 = \gamma_0(M', \omega') > 0$, independent of h and $|V|$, such that

$$\sum_{|\alpha| \leq 2} (|\partial^\alpha(u_h - u)(x)| + |\partial^\alpha(\phi_h - \phi)(x)|) + |(m_h - m)(x)| \leq C h e^{-\gamma_0|x - Y_k|}, \quad (6.94)$$

$$\|u_h - u\|_{H^4(\mathbb{R}^3)} + \|\phi_h - \phi\|_{H^2(\mathbb{R}^3)} \leq C \|m_h - m\|_{L^2(\mathbb{R}^3)} \leq C h. \quad (6.95)$$

Moreover, the limits

$$\bar{u} = \lim_{h \rightarrow 0} \frac{u_h - u}{h}, \quad \bar{\phi} = \lim_{h \rightarrow 0} \frac{\phi_h - \phi}{h}, \quad \bar{m} = \lim_{h \rightarrow 0} \frac{m_h - m}{h},$$

exist and are the unique solution to the linearised TFW equations

$$-\Delta \bar{u} + \left(\frac{35}{9} u^{4/3} - \phi \right) \bar{u} - u \bar{\phi} = 0, \quad (6.96a)$$

$$-\Delta \bar{\phi} = 4\pi (\bar{m} - 2u\bar{u}). \quad (6.96b)$$

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

$$\sum_{|\alpha| \leq 2} (|\partial^\alpha \bar{u}(x)| + |\partial^\alpha \bar{\phi}(x)|) + |\bar{m}(x)| \leq C e^{-\gamma_0|x - Y_k|}, \quad (6.97)$$

$$\|\bar{u}\|_{H^4(\mathbb{R}^3)} + \|\bar{\phi}\|_{H^2(\mathbb{R}^3)} \leq C \|\bar{m}\|_{L^2(\mathbb{R}^3)}. \quad (6.98)$$

Proof (Proof of Lemma 6.7). By Propositions 3.1 and 3.2, for $h \in [0, h_0]$ the ground state (u_h, ϕ_h) satisfies

$$\|u_h\|_{H_{\text{unif}}^4(\mathbb{R}^3)} + \|\phi_h\|_{H_{\text{unif}}^2(\mathbb{R}^3)} \leq C(M'), \quad (6.99)$$

$$\inf_{x \in \mathbb{R}^3} u_h(x) \geq c_{M', \omega'} > 0, \quad (6.100)$$

independently of h . From (6.93), it follows that

$$\begin{aligned} |(m_h - m)(x)| &= |\eta(x - Y_k - hV) - \eta(x - Y_k)| \\ &\leq h|V| \int_0^1 |\nabla \eta(x - Y_k - thV)| \, dt \\ &\leq \int_0^1 |\nabla \eta(x - Y_k - thV)| \, dt. \end{aligned} \quad (6.101)$$

For all $h \in [0, h_0]$, $\text{spt}(m_h - m) \subset B_{R_0+1}(Y_k)$, so by Corollary 4.1 and (6.101) it follows that there exists $\gamma_0 > 0$ such that

$$\sum_{|\alpha| \leq 2} |\partial^\alpha (u_h - u)(x)| + |(\phi_h - \phi)(x)| + |(m_h - m)(x)| \leq C h e^{-\gamma_0 |x - Y_k|}, \quad (6.102)$$

and (6.95) holds

$$\|u_h - u\|_{H^4(\mathbb{R}^3)} + \|\phi_h - \phi\|_{H^2(\mathbb{R}^3)} \leq C \|m_h - m\|_{L^2(\mathbb{R}^3)} \leq Ch. \quad (6.103)$$

Due to the uniform estimates (6.99)–(6.100) and (6.101), the constants appearing on the right-hand side are independent of h .

We now show

$$\sum_{|\alpha| \leq 2} |\partial^\alpha (\phi_h - \phi)(x)| \leq C e^{-\gamma_0 |x - Y_k|}. \quad (6.104)$$

Observe that for $h \in (0, h_0]$ as $\text{spt}(m_h - m) \subset B_{R_0+1}(Y_k)$, by the triangle inequality $x \in B_{R_0+3}^c(Y_k)$ implies $B_2(x) \subset B_{R_0+1}^c(Y_k)$. Consequently, for $x \in B_{R_0+3}^c(Y_k)$

$$\|m_h - m\|_{C^{0,1/2}(B_2(x))} = 0, \quad (6.105)$$

and for $x \in B_{R_0+3}(Y_k)$, by (6.93) it follows that

$$\|m_h - m\|_{C^{0,1/2}(B_2(x))} \leq 2 \|\eta\|_{C^{0,1/2}(B_2(x))}. \quad (6.106)$$

By (6.105)–(6.106) we deduce that $x \mapsto \|m_h - m_0\|_{C^{0,1/2}(B_2(x))}$ is a bounded function with support in $B_{R_0+3}(Y_k)$, hence there exists $C > 0$ such that

$$\|m_h - m\|_{C^{0,1/2}(B_2(x))} \leq C e^{-\gamma_0 |x - Y_k|}. \quad (6.107)$$

Then we apply the Schauder estimates [26, Theorem 10.2.1, Lemma 10.1.1] together with (6.102) and (6.107) to estimate

$$\begin{aligned}
 \|\phi_h - \phi\|_{C^{2,1/2}(B_1(x))} &\leq C \left(\|m_h - m - u_h^2 + u^2\|_{C^{0,1/2}(B_2(x))} + \|\phi_h - \phi\|_{L^2(B_2(x))} \right), \\
 &\leq C \left(\|m_h - m\|_{C^{0,1/2}(B_2(x))} + \|u_h^2 - u^2\|_{C^{0,1/2}(B_2(x))} \right. \\
 &\quad \left. + \|\phi_h - \phi\|_{L^2(B_2(x))} \right), \\
 &\leq C \left(\|(u_h + u)(u_h - u)\|_{C^{0,1/2}(B_2(x))} + e^{-\gamma_0|x-Y_k|} \right), \\
 &\leq C \left(\|u_h + u\|_{C^{0,1/2}(B_2(x))} \|u_h - u\|_{C^{0,1/2}(B_2(x))} + e^{-\gamma_0|x-Y_k|} \right).
 \end{aligned} \tag{6.108}$$

Applying the Sobolev embedding $C^{0,1/2}(B_2(x)) \hookrightarrow H^2(B_2(x))$ and using (6.100), it follows that

$$\|u_h + u\|_{C^{0,1/2}(B_2(x))} \leq C \|u_h + u\|_{H^2(B_2(x))} \leq C \left(\|u_h\|_{H_{\text{unif}}^2(\mathbb{R}^3)} + \|u\|_{H_{\text{unif}}^2(\mathbb{R}^3)} \right) \leq C. \tag{6.109}$$

Applying (6.109) and (6.102) to (6.108), we obtain the desired estimate (6.104): for any multi-index α satisfying $|\alpha| \leq 2$

$$\begin{aligned}
 |\partial^\alpha(\phi_h - \phi)(x)| &\leq \|\phi_h - \phi\|_{W^{2,\infty}(B_1(x))} \leq \|\phi_h - \phi\|_{C^{2,1/2}(B_1(x))} \\
 &\leq C \left(\|u_h + u\|_{C^{0,1/2}(B_2(x))} \|u_h - u\|_{C^{0,1/2}(B_2(x))} + e^{-\gamma_0|x-Y_k|} \right) \\
 &\leq C \left(\|u_h - u\|_{W^{1,\infty}(B_2(x))} + e^{-\gamma_0|x-Y_k|} \right) \leq C e^{-\gamma_0|x-Y_k|}.
 \end{aligned} \tag{6.110}$$

We will show next that there exist $\bar{u} \in H^4(\mathbb{R}^3)$, $\bar{\phi} \in H^2(\mathbb{R}^3)$ such that $\frac{u_h - u}{h}$, $\frac{\phi_h - \phi}{h}$ converge to \bar{u} , $\bar{\phi}$ 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 as $h \rightarrow 0$.

First consider any decreasing sequence $h_n \rightarrow 0$, then there exists a subsequence (still denoted by h_n) such that $\frac{u_{h_n} - u}{h_n}$, $\frac{\phi_{h_n} - \phi}{h_n}$ converge to $\bar{u} \in H^4(\mathbb{R}^3)$, $\bar{\phi} \in H^2(\mathbb{R}^3)$ 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 $(\bar{u}, \bar{\phi})$ satisfy (6.97)–(6.98).

We now verify that the limiting functions are independent of the choice of sequence. First, observe that by passing to the limit as $h_n \rightarrow 0$ in the equations

$$\begin{aligned}
 -\Delta \left(\frac{u_{h_n} - u}{h_n} \right) + \frac{5}{3} \frac{u_{h_n}^{7/3} - u^{7/3}}{h_n} - \frac{\phi_{h_n} u_{h_n} - \phi u}{h_n} &= 0, \\
 -\Delta \left(\frac{\phi_{h_n} - \phi}{h_n} \right) &= 4\pi \left(\frac{m_{h_n} - m}{h_n} - \frac{u_{h_n}^2 - u^2}{h_n} \right),
 \end{aligned}$$

it follows that $(\bar{u}, \bar{\phi})$ solve the linearised TFW equations (6.96) pointwise,

$$\begin{aligned} -\Delta \bar{u} + \left(\frac{35}{9} u^{4/3} - \phi \right) \bar{u} - u \bar{\phi} &= 0, \\ -\Delta \bar{\phi} &= 4\pi (\bar{m} - 2u\bar{u}), \\ \text{where } \bar{m}(x) &= \lim_{h_n \rightarrow 0} \frac{(m_{h_n} - m)(x)}{h_n} = -\nabla \eta(x - Y_k) \cdot V. \end{aligned}$$

Clearly \bar{m} is independent of the sequence h_n . Applying [7, Corollary 2.3], it follows that the $(\bar{u}, \bar{\phi})$ is the unique solution to the linearised system (6.96), hence is independent of the sequence (h_n) . It then follows that $\frac{u_h - u}{h}$, $\frac{\phi_h - \phi}{h}$ converge to \bar{u} , $\bar{\phi}$ as $h \rightarrow 0$ as stated above. \square

We are now in a position to prove Theorem 4.2.

Proof (Proof of Theorem 4.2). We will repeatedly use the fact that there exists $C, \gamma > 0$ such that, for all $h \in [0, h_0]$, $p \in [1, 2]$,

$$\int_{\mathbb{R}^3} (1 + m_h(x) + |\nabla \phi_h(x)|)^p e^{-\gamma_0|x-Y_k|} e^{-\tilde{\gamma}|x-Y_j|} dx \leq C e^{-\gamma|Y_j-Y_k|}, \quad (6.111)$$

which is a consequence of the uniform bounds on m_h , ϕ_h and of (6.86).

Further, we require that there exist $C, \tilde{\gamma} > 0$ such that, for $j \in \mathbb{N}$, $h \in (0, h_0]$, $x \in \mathbb{R}^3$,

$$\left| \frac{\varphi_j(Y^h; x) - \varphi_j(Y; x)}{h} \right| \leq C e^{-\tilde{\gamma}|x-Y_j|} e^{-\tilde{\gamma}|x-Y_k|}, \quad (6.112)$$

which follows directly from (4.19c).

For $i = 1, 2$ and $j \in \mathbb{N}$, consider the difference

$$\begin{aligned} \frac{E_j^i(Y^h) - E_j^i(Y)}{h} &= \int_{\mathbb{R}^3} \frac{\mathcal{E}_i(Y^h; x) \varphi_j(Y^h; x) - \mathcal{E}_i(Y; x) \varphi_j(Y; x)}{h} dx \\ &= \int_{\mathbb{R}^3} \left(\frac{\mathcal{E}_i(Y^h; x) - \mathcal{E}_i(Y; x)}{h} \right) \varphi_j(Y^h; x) dx \\ &\quad + \int_{\mathbb{R}^3} \mathcal{E}_i(Y; x) \left(\frac{\varphi_j(Y^h; x) - \varphi_j(Y; x)}{h} \right) dx \end{aligned} \quad (6.113)$$

We wish to show that the limit of (6.113) exists as $h \rightarrow 0$ to obtain

$$\frac{\partial E_j^i}{\partial Y_k} = \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_i}{\partial Y_k}(Y; x) \varphi_j(Y; x) dx + \int_{\mathbb{R}^3} \mathcal{E}_i(Y; x) \frac{\partial \varphi_j}{\partial Y_k}(Y; x) dx, \quad (6.114)$$

where

$$\frac{\partial \mathcal{E}_1}{\partial Y_k}(Y; \cdot) = 2\nabla u \cdot \nabla \bar{u} + \frac{10}{3} u^{7/3} \bar{u} + \frac{1}{2} \bar{\phi} (m - u^2) + \frac{1}{2} \phi (\bar{m} - 2u\bar{u}), \quad (6.115)$$

$$\frac{\partial \mathcal{E}_2}{\partial Y_k}(Y; \cdot) = 2\nabla u \cdot \nabla \bar{u} + \frac{10}{3} u^{7/3} \bar{u} + \frac{1}{4\pi} \nabla \bar{\phi} \cdot \nabla \phi. \quad (6.116)$$

Case 1. First consider the energy density

$$\mathcal{E}_1(Y; x) = |\nabla u(x)|^2 + u^{10/3}(x) + \frac{1}{2}\phi(x)(m - u^2)(x). \quad (6.117)$$

To show (6.115), consider the difference

$$\begin{aligned} \frac{\mathcal{E}_1(Y^h; \cdot) - \mathcal{E}_1(Y; \cdot)}{h} &= \nabla(u_h + u) \cdot \nabla \left(\frac{u_h - u}{h} \right) + \left(\frac{u_h^{10/3} - u^{10/3}}{h} \right) \\ &\quad + \frac{1}{2h} \left(\phi_h(m_h - u_h^2) - \frac{1}{2}\phi(m - u^2) \right) \\ &= \nabla(u_h + u) \cdot \nabla \left(\frac{u_h - u}{h} \right) + \left(\frac{u_h^{10/3} - u^{10/3}}{h} \right) \\ &\quad + \frac{1}{2} \left(\frac{\phi_h - \phi}{h} \right) (m - u^2) + \frac{1}{2}\phi_h \left(\frac{m_h - m - u_h^2 + u^2}{h} \right). \end{aligned} \quad (6.118)$$

It follows from (6.118) and pointwise convergence of $u_h, \nabla u_h, \phi_h$ to $u, \nabla u, \phi$ and $\frac{u_h - u}{h}, \nabla \left(\frac{u_h - u}{h} \right), \frac{\phi_h - \phi}{h}, \frac{m_h - m}{h}$ to $\bar{u}, \nabla \bar{u}, \bar{\phi}, \bar{m}$ as $h \rightarrow 0$, that (6.115) holds

$$\lim_{h \rightarrow 0} \frac{\mathcal{E}_1(Y^h; \cdot) - \mathcal{E}_1(Y; \cdot)}{h} = 2\nabla u \cdot \nabla \bar{u} + \frac{10}{3}u^{7/3}\bar{u} + \frac{1}{2}\bar{\phi}(m - u^2) + \frac{1}{2}\phi(\bar{m} - 2u\bar{u}) = \frac{\partial \mathcal{E}_1}{\partial Y_k}.$$

Applying (6.94) to (6.118) yields

$$\begin{aligned} \left| \mathcal{E}_1(Y^h; x) - \mathcal{E}_1(Y; x) \right| &\leq C(|(u_h - u)(x)| + |\nabla(u_h - u)(x)| + |(m_h - m)(x)|) \\ &\quad + C(1 + m(x))|(\phi_h - \phi)(x)| \\ &\leq Ch(1 + m(x))e^{-\gamma_0|x - Y_k|}. \end{aligned} \quad (6.119)$$

Combining (6.119) and (4.19b), we deduce

$$\left| \frac{\mathcal{E}_1(Y^h; x) - \mathcal{E}_1(Y; x)}{h} \varphi_j(Y; x) \right| \leq C(1 + m(x))e^{-\gamma_0|x - Y_k|}e^{-\tilde{\gamma}|x - Y_j|}, \quad (6.120)$$

hence by (6.111) and the Dominated Convergence Theorem,

$$\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_1}{\partial Y_k}(Y; x) \varphi_j(Y; x) \, dx = \lim_{h \rightarrow 0} \int_{\mathbb{R}^3} \left(\frac{\mathcal{E}_1(Y^h; x) - \mathcal{E}_1(Y; x)}{h} \right) \varphi_j(Y; x) \, dx. \quad (6.121)$$

It follows from (6.120) and (6.111) that

$$\left| \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_1}{\partial Y_k}(Y; x) \varphi_j(Y; x) \, dx \right| \leq C \int_{\mathbb{R}^3} (1 + m(x))e^{-\gamma_0|x - Y_k|}e^{-\tilde{\gamma}|x - Y_j|} \, dx \leq Ce^{-\gamma|Y_j - Y_k|}. \quad (6.122)$$

It remains to show that (6.113) converges using (6.111) and (6.112). As $\varphi_j(Y; x)$ is differentiable with respect to Y_k , for all $x \in \mathbb{R}^3$

$$\mathcal{E}_1(Y; x) \frac{\partial \varphi_j}{\partial Y_k}(Y; x) = \lim_{h \rightarrow 0} \mathcal{E}_1(Y; x) \left(\frac{\varphi_j(Y^h; x) - \varphi_j(Y; x)}{h} \right),$$

and combining (6.117) with (6.112) implies

$$\left| \mathcal{E}_1(Y; x) \left(\frac{\varphi_j(Y^h; x) - \varphi_j(Y; x)}{h} \right) \right| \leq C(1 + m(x))e^{-\gamma_0|x-Y_k|}e^{-\tilde{\gamma}|x-Y_j|},$$

hence by (6.111) and the Dominated Convergence Theorem,

$$\begin{aligned} \int_{\mathbb{R}^3} \mathcal{E}_1(Y; x) \frac{\partial \varphi_j}{\partial Y_k}(Y; x) dx &= \lim_{h \rightarrow 0} \int_{\mathbb{R}^3} \mathcal{E}_1(Y; x) \left(\frac{\varphi_j(Y^h; x) - \varphi_j(Y; x)}{h} \right) dx, \\ \text{and } \left| \int_{\mathbb{R}^3} \mathcal{E}_1(Y; x) \frac{\partial \varphi_j}{\partial Y_k}(Y; x) dx \right| &\leq C e^{-\gamma|Y_j-Y_k|}. \end{aligned} \quad (6.123)$$

Combining (6.122) and (6.123) yields the desired estimate (4.21).

The second case, using \mathcal{E}_2 instead of \mathcal{E}_1 , is analogous. \square

Proof (Proof of (4.22)). We will use

$$\sum_{j \in \mathbb{N}} e^{-\gamma|Y_j-Y_k|} < \infty, \quad (6.124)$$

which is a consequence of (H1) and that $Y \in \mathcal{D}_{L^2}(M, \omega)$. Then for $i \in \{1, 2\}$

$$\begin{aligned} \sum_{j \in \mathbb{N}} \left| \frac{\partial E_j^i}{\partial Y_k} \right| &\leq \sum_{j \in \mathbb{N}} \left| \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_i}{\partial Y_k}(Y; x) \varphi_j(Y; x) dx \right| + \sum_{j \in \mathbb{N}} \left| \int_{\mathbb{R}^3} \mathcal{E}_i(Y; x) \frac{\partial \varphi_j}{\partial Y_k}(Y; x) dx \right| \\ &\leq C \sum_{j \in \mathbb{N}} e^{-\gamma|Y_j-Y_k|} < \infty, \end{aligned}$$

hence by the Monotone Convergence Theorem, the sum is well-defined

$$\sum_{j \in \mathbb{N}} \frac{\partial E_j^1}{\partial Y_k} = \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_1}{\partial Y_k}(Y; x) \left(\sum_{j \in \mathbb{N}} \varphi_j(Y; x) \right) dx + \int_{\mathbb{R}^3} \mathcal{E}_1(Y; x) \left(\sum_{j \in \mathbb{N}} \frac{\partial \varphi_j}{\partial Y_k}(Y; x) \right) dx.$$

As $(\varphi_j)_{j \in \mathbb{N}}$ satisfies (4.19a) for all $h \in [0, h_0]$, it follows that

$$\sum_{j \in \mathbb{N}} \frac{\partial \varphi_j}{\partial Y_k}(Y; x) = 0,$$

and consequently,

$$\sum_{j \in \mathbb{N}} \frac{\partial E_j^1}{\partial Y_k} = \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_1}{\partial Y_k}(Y; x) dx.$$

Now consider the difference of (6.115)–(6.116)

$$\left(\frac{\partial \mathcal{E}_1}{\partial Y_k} - \frac{\partial \mathcal{E}_2}{\partial Y_k} \right) (Y; \cdot) = \frac{1}{2} \bar{\phi}(m - u^2) + \frac{1}{2} \phi(\bar{m} - 2u\bar{u}) - \frac{1}{4\pi} \nabla \bar{\phi} \cdot \nabla \phi, \quad (6.125)$$

and applying integration by parts yields

$$\begin{aligned} \int_{\mathbb{R}^3} \left(\frac{\partial \mathcal{E}_1}{\partial Y_k} - \frac{\partial \mathcal{E}_2}{\partial Y_k} \right) (Y; x) \, dx &= \int_{\mathbb{R}^3} \left(\frac{1}{2} \bar{\phi}(m - u^2) + \frac{1}{2} \phi(\bar{m} - 2u\bar{u}) - \frac{1}{4\pi} \nabla \bar{\phi} \cdot \nabla \phi \right) \\ &= \frac{1}{8\pi} \int_{\mathbb{R}^3} (\bar{\phi}(-\Delta \phi) + \phi(-\Delta \bar{\phi}) - 2\nabla \bar{\phi} \cdot \nabla \phi) \\ &= \frac{1}{8\pi} \int_{\mathbb{R}^3} (2\nabla \bar{\phi} \cdot \nabla \phi - 2\nabla \bar{\phi} \cdot \nabla \phi) = 0. \end{aligned}$$

In addition, since

$$\frac{1}{4\pi} \int_{\mathbb{R}^3} \nabla \phi \cdot \nabla \bar{\phi} = \frac{1}{4\pi} \int_{\mathbb{R}^3} \phi(-\Delta \bar{\phi}) = \int_{\mathbb{R}^3} \phi(\bar{m} - 2u\bar{u})$$

and since u solves (2.6a), $-\Delta u + \frac{5}{3}u^{7/3} - \phi u = 0$, the desired result (4.22) holds:

$$\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_2}{\partial Y_k} (Y; x) \, dx = 2 \int_{\mathbb{R}^3} \left(\nabla u \cdot \nabla \bar{u} + \frac{5}{3} u^{7/3} \bar{u} - \phi u \bar{u} \right) + \int_{\mathbb{R}^3} \phi \bar{m} = \int_{\mathbb{R}^3} \phi \bar{m}.$$

□

Finally, we establish (4.16)–(4.17): if the partition functions φ_j are invariant under permutations and isometries, then so are the site energies.

Lemma 6.8. *If the partition $(\varphi_j)_{j \in \mathbb{N}}$ is permutation and isometry invariant (4.23)–(4.24), then for $i = 1, 2$, for any bijection $P : \mathbb{N} \rightarrow \mathbb{N}$, isometry $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$, $j \in \mathbb{N}$ and $Y \in \mathcal{Y}_{L^2}(M, \omega)$*

$$E_j^i(Y \circ P) = E_j^i(Y), \quad (6.126)$$

$$E_j^i(AY) = E_j^i(Y). \quad (6.127)$$

Proof (Proof of Lemma 6.8). Let $Y \in \mathcal{Y}_{L^2}(M, \omega)$ and $m = m_Y$, then as $P : \mathbb{N} \rightarrow \mathbb{N}$ is a bijection,

$$m_{Y \circ P}(x) = \sum_{j \in \mathbb{N}} \eta(x - Y_{P_j}) = \sum_{j \in \mathbb{N}} \eta(x - Y_j) = m_Y(x).$$

Since (2.6) has a unique solution, $(u_Y, \phi_Y) = (u_{Y \circ P}, \phi_{Y \circ P})$. Consequently, the energy densities agree, $\mathcal{E}_i(Y \circ P; \cdot) = \mathcal{E}_i(Y; \cdot)$. Together with (4.23) this implies (6.126).

We now show isometry invariance (6.127). First consider a translation $A_1(x) = x + c$, for $c \in \mathbb{R}^3$, then

$$m_{A_1 Y}(x) = \sum_{j \in \mathbb{N}} \eta(x - Y_j - c) = m_Y(x - c) = m_Y(A_1^{-1}(x)).$$

Then, by the uniqueness of the TFW equations, it follows that $(u_{A_1 Y}, \phi_{A_1 Y})(\cdot) = (u_Y, \phi_Y)(\cdot - c)$, so $\mathcal{E}_i(A_1 Y; \cdot) = \mathcal{E}_i(Y; \cdot - c)$ and thus

$$\begin{aligned} E_j^i(A_1 Y) &= \int_{\mathbb{R}^3} \mathcal{E}_i(A_1 Y; x) \varphi_j(A_1 Y; x) \, dx = \int_{\mathbb{R}^3} \mathcal{E}_i(Y; x - c) \varphi_j(Y; x - c) \, dx \\ &= \int_{\mathbb{R}^3} \mathcal{E}_i(Y; z) \varphi_j(Y; z) \, dz = E_j^i(Y). \end{aligned}$$

Similarly, for a rotation $A_2(x) = Rx$, $R \in O(3)$, since we assumed that η is radially symmetric,

$$m_{A_2 Y}(x) = \sum_{j \in \mathbb{N}} \eta(x - RY_j) = \sum_{j \in \mathbb{N}} \eta(R(R^T x - Y_j)) = \sum_{j \in \mathbb{N}} \eta(R^T x - Y_j) = m_Y(R^T x). \quad (6.128)$$

As (u_Y, ϕ_Y) solve (2.6)

$$\begin{aligned} -\Delta u_Y + \frac{5}{3} u_Y^{7/3} - \phi_Y u_Y &= 0, \\ -\Delta \phi_Y &= 4\pi(m_Y - u_Y^2), \end{aligned}$$

then by (6.128) and as the Laplacian is invariant under rotations, it follows that $(u, \phi) = (u_Y, \phi_Y) \circ A_2^{-2}$ solves

$$\begin{aligned} -\Delta u + \frac{5}{3} u^{7/3} - \phi u &= 0, \\ -\Delta \phi &= 4\pi(m_Y \circ R^T - u^2) = 4\pi(m_{A_2 Y} - u^2), \end{aligned}$$

hence the uniqueness of (2.6) implies $(u_{A_2 Y}, \phi_{A_2 Y}) = (u_Y, \phi_Y) \circ A_2^{-1}$. It follows that $E_i(A_2 Y; \cdot) = E_i(Y; R^T \cdot)$, hence as $\det(R) = 1$, a change of variables shows

$$\begin{aligned} E_j^i(A_2 Y) &= \int_{\mathbb{R}^3} \mathcal{E}_i(A_2 Y; x) \varphi_j(A_2 Y; x) \, dx = \int_{\mathbb{R}^3} \mathcal{E}_i(Y; R^T x) \varphi_j(Y; R^T x) \, dx \\ &= \int_{\mathbb{R}^3} \mathcal{E}_i(Y; z) \varphi_j(Y; z) |\det(R)| \, dz = \int_{\mathbb{R}^3} \mathcal{E}_i(Y; z) \varphi_j(Y; z) \, dz = E_j^i(Y). \end{aligned}$$

As the site energies are invariant under both translations and rotations, they are invariant under all isometries of \mathbb{R}^3 . \square

Acknowledgements. We thank Chen Huang for his valuable comments on impurity screening in the Thomas–Fermi model, and Eric Cancès and Virginie Ehrlacher for helpful discussions about different analytical techniques for the TFW model.

Open Access This article is distributed under the terms of the Creative Commons Attribution 4.0 International License (<http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted use, distribution, and reproduction in any medium, provided you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made.

References

1. AGMON, S.: *Lectures on the Exponential Decay of Solutions of Second-Order Elliptic Equations: Bounds on Eigenfunctions of N-Body Schrödinger Operations (MN-29)*. Princeton University Press (2014)
2. ASHCROFT, N., MERMIN, N.: *Solid State Physics*. Saunders College, Rochester, 1976
3. AUBIN, T.: *Nonlinear Analysis on Manifolds. Monge–Ampère Equations*, Vol. 252. Springer, Berlin, 1982
4. BADER, R.: *Atoms in Molecules*. Wiley Online Library, New York, 1990
5. BENGURIA, R., BRÉZIS, H., LIEB, E.: The Thomas–Fermi–von Weizsäcker theory of atoms and molecules. *Commun. Math. Phys.* **79**(2), 167–180, 1981
6. BENZI, M., BOITO, P., RAZOUK, N.: Decay properties of spectral projectors with applications to electronic structure. *SIAM Rev.* **55**(1), 3–64, 2013
7. BLANC, X.: Unique solvability of a system of nonlinear elliptic pdes arising in solid state physics. *SIAM J. Math. Anal.* **38**(4), 1235–1248, 2006
8. BLANC, X., MONNEAU, R.: Screening of an applied electric field inside a metallic layer described by the Thomas–Fermi–von Weizsäcker model. *Adv. Differ. Equ.* **7**(7), 847–876, 2002
9. BRÉZIS, H., LIEB, E.: Long range atomic potentials in Thomas–Fermi theory. *Commun. Math. Phys.* **65**(3), 231–246, 1979
10. CANCÈS, E., EHRLACHER, V.: Local defects are always neutral in the Thomas–Fermi–von Weizsäcker theory of crystals. *Arch. Ration. Mech. Anal.* **202**(3), 933–973, 2011
11. CANCÈS, E., LEWIN, M.: The dielectric permittivity of crystals in the reduced Hartree–Fock approximation. *Arch. Ration. Mech. Anal.* **197**(1), 139–177, 2010
12. CATTO, I., LE BRIS, C., LIONS, P.-L.: *The Mathematical Theory of Thermodynamic Limits: Thomas–Fermi Type Models*. Oxford Mathematical Monographs. The Clarendon Press, Oxford University Press, New York, 1998
13. CHEN, H., NAZAR, F., ORTNER, C.: Models for crystalline defects (**in preparation**)
14. CHEN, H., ORTNER, C.: QMMM methods for crystalline defects. Part 1: Locality of the tight binding model. *Multiscale Model. Simul.* **14**(1), 232–264 (2015)
15. CHEN, H., ORTNER, C.: QMMM methods for crystalline defects. Part 2: Consistent energy and force-mixing. *Multiscale Model. Simul.* **15**(1), 184–214 (2017)
16. COMBES, J.-M., THOMAS, L.: Asymptotic behaviour of eigenfunctions for multiparticle Schrödinger operators. *Commun. Math. Phys.* **34**(4), 251–270, 1973
17. CSÁNYI, G., ALBARET, T., MORAS, G., PAYNE, M., DE VITA, A.: Multiscale hybrid simulation methods for material systems. *J. Phys. Condens. Matter* **17**(27), R691, 2005
18. DONOVAN, B., MARCH, N.: Screening of point singularities in metals, with particular reference to positron annihilation. *J. Phys. Chem. Solids* **11**(1–2), 68–72, 1959
19. EHRLACHER, V., ORTNER, C., SHAPEEV, A.: Analysis of boundary conditions for crystal defect atomistic simulations. 2013. [arXiv:1306.5334](https://arxiv.org/abs/1306.5334)
20. EVANS, L.: *Partial Differential Equations, Volume 19 of Graduate Studies in Mathematics*, 2nd edn. American Mathematical Society, Providence, 2010
21. EVANS, L., GARIEPY, R.: *Measure Theory and Fine Properties of Functions*, Vol. 5. CRC Press, Boca Raton, 1991
22. GABOVICH, A., IL'CHENKO, L., PASHITSKII, E., ROMANOV, Y.: Screening of charges and Friedel oscillations of the electron density in metals having differently shaped Fermi surfaces. *Sov. J. Exp. Theor. Phys.* **48**, 124, 1978
23. GILBARG, D., TRUDINGER, N.: *Elliptic Partial Differential Equations of Second Order*. Classics in Mathematics. Springer, Berlin, 2001 (reprint of the 1998 edition)
24. GOEDECKER, S.: Linear scaling electronic structure methods. *Rev. Mod. Phys.* **71**, 1085–1123, 1999
25. ISMAIL-BEIGI, S., ARIAS, T.: Locality of the density matrix in metals, semiconductors, and insulators. 1999. [arXiv:cond-mat.mtrl-sci/9805147v4](https://arxiv.org/abs/cond-mat.mtrl-sci/9805147v4)
26. JOST, J.: *Partial Differential Equations, Volume 214 of Graduate Texts in Mathematics*, 3rd edn. Springer, New York, 2013

27. POOLE, JR, C.: *Encyclopedic Dictionary of Condensed Matter Physics*, Vol. 1. Academic Press, Cambridge, 2004
28. KITTEL, C., FONG, C.-Y.: *Quantum Theory of Solids*. Wiley, New York, 1963
29. LADÁNYI, K., NAGY, I., APAGYI, B.: Partially linearized Thomas–Fermi–Weizsäcker theory for screening and stopping of charged particles in jellium. *Phys. Rev. A* **45**, 2989–2997, 1992
30. LIEB, E., SIMON, B.: The Thomas–Fermi theory of atoms, molecules and solids. *Adv. Math.* **23**(1), 22–116, 1977
31. LIEB, E.H.: Thomas–Fermi and related theories of atoms and molecules. *Rev. Mod. Phys.* **53**, 603–641, 1981
32. MARCH, N.: *Electron Density Theory of Atoms and Molecules*. Academic Press, Cambridge, 1992
33. MARCH, N., YOUNG, W.H., SAMPANTHAR, S.: *The Many-Body Problem in Quantum Mechanics*. Courier Corporation, Mineola, 1967
34. MARKOWICH, P., RINGHOFER, C., SCHMEISER, C.: *Semiconductor Equations*. Springer, New York, 1990
35. NAGY, I., ARNAU, A., ECHENIQUE, M., LADÁNYI, K.: Stopping power of a finite-temperature electron gas for slow unit charges. *Phys. Rev. A* **43**, 6038–6042, 1991
36. NAZAR, F.Q.: Convergence rates from Yukawa to Coulomb interaction in the Thomas–Fermi–von Weizsäcker model. 2016. [arXiv:1601.01187](https://arxiv.org/abs/1601.01187)
37. ORTNER, C., THEIL, F.: Justification of the Cauchy–Born approximation of elastodynamics. *Arch. Ration. Mech. Anal.* **207**, 2013
38. PRODAN, E., KOHN, W.: Nearsightedness of electronic matter. *Proce. Natl. Acad. Sci. USA* **102**(33), 11635–11638, 2005
39. RESTA, R.: Thomas–Fermi dielectric screening in semiconductors. *Phys. Rev. B* **16**(6), 2717, 1977
40. SCARFONE, L.: Weizsäcker correction in the Thomas–Fermi and Thomas–Fermi–Dirac models of static dielectric screening in undoped semiconductors: Impurity donor ions in silicon and germanium. *Phys. Rev. B* **45**, 8348–8354, 1992
41. SOLOVEJ, J.: Universality in the Thomas–Fermi–von Weizsäcker model of atoms and molecules. *Commun. Math. Phys.* **129**(3), 561–598, 1990
42. TRUDINGER, N.: Linear elliptic operators with measurable coefficients. *Annali della Scuola Normale Superiore di Pisa-Classe di Scienze* **27**(2), 265–308, 1973
43. WANG, Z., ZHOU, H.: Positive solution for a nonlinear stationary Schrödinger–Poisson system in \mathbb{R}^3 . *Discrete Contin. Dyn. Syst.* **18**(4), 809, 2007
44. YU, M., TRINKLE, D., MARTIN, R.: Energy density in density functional theory: application to crystalline defects and surfaces. *Phys. Rev. B* **83**(11), 115113, 2011
45. ZHAO, L., ZHAO, F.: On the existence of solutions for the Schrödinger–Poisson equations. *J. Math. Anal. Appl.* **346**(1), 155–169, 2008

F. Q. NAZAR

Mathematics Institute, Zeeman Building,
University of Warwick,
Coventry CV4 7AL, UK.
e-mail: F.Q.Nazar@warwick.ac.uk

and

C. ORTNER

Mathematics Institute, Zeeman Building,
University of Warwick,
Coventry CV4 7AL, UK.
e-mail: C.Ortner@warwick.ac.uk

(Received September 22, 2015 / Accepted January 5, 2017)
Published online February 21, 2017 – © The Author(s) (2017)
This article is published with open access at Springerlink.com