Locality of the TFW Equations

Faizan Nazar

Applied PDE Seminar, University of Warwick

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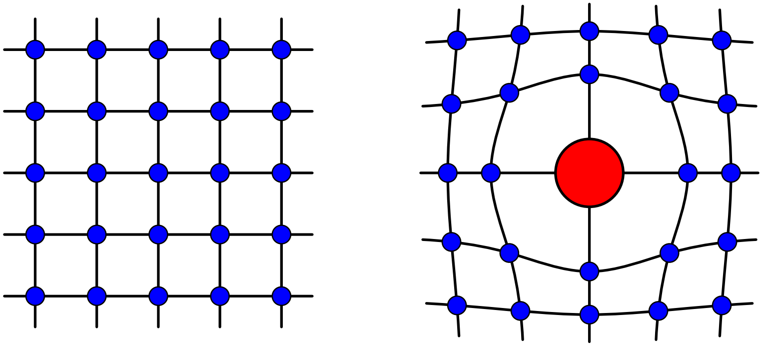
Mathematics and Statistics
Centre for Doctoral Training

Motivation



$$\mathcal{I} = \inf\{\, \mathcal{E}(U_\Lambda) \mid U_\Lambda \in \mathcal{U}^{1,2} \,\}, \quad \mathcal{I}^{d} = \inf\{\, \mathcal{E}^{d}(U_\Lambda) \mid U_\Lambda \in \mathcal{U}^{1,2} \,\}.$$

Motivation - Existing Work

- [Cances, Ehrlacher (2011)] - Local defects are always neutral in the Thomas-Fermi-von Weizsäcker theory of crystals, *Arch. Rational Mech. Anal.*

- [Ehrlacher, Ortner, Shapeev (2013)] - Analysis of Boundary Conditions for Crystal Defect Atomistic Simulations, *Preprint.*

- [Catto, Le Bris, Lions (1998)] - The Mathematical Theory of Thermodynamic Limits: Thomas–Fermi Type Models, *Oxford Mathematical Monographs.*

Outline

- Introduction
- Uniform Regularity Estimates
- Pointwise Stability Estimates
- Applications
- Outlook

The TFW Model

Let $u, m : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ denote

- u - square root of the electron density,
- m - nuclear distribution,
- ϕ - potential generated by u and m, which solves

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

The Thomas-Fermi-von Weizsäcker functional is then defined by

$$E^{TFW}(u, m) = \int_{\mathbb{R}^3} |\nabla u|^2 + \int_{\mathbb{R}^3} u^{10/3} + \frac{1}{2} D(m - u^2, m - u^2),$$

where

$$D(f, g) = \int\int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(x)g(y)}{|x - y|} \, \mathrm{d}x \, \mathrm{d}y.$$

For finite systems, with $u \in H^1(\mathbb{R}^3)$ and $m \in L^{6/5}(\mathbb{R}^3)$, this is well-defined.

Existence and Uniqueness of Solutions

Theorem (Catto, Le Bris, Lions (1998))

Let m be a non-negative function satisfying:

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

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

then there exists a unique distributional solution (u, ϕ) *to*

$$-\Delta u + \frac{5}{3} u^{7/3} - \phi u = 0, \quad (1)$$

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

satisfying $u \in H^2_{\mathrm{unif}}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3), \inf u > 0, \phi \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$.

where $\|f\|_{L^2_{unif}(\mathbb{R}^3)} = \sup_{x\in\mathbb{R}^3} \|f\|_{L^2(B_1(x))}, \|f\|_{H^2_{unif}(\mathbb{R}^3)} = \sup_{x\in\mathbb{R}^3} \|f\|_{H^2(B_1(x))}$.

Nuclear Configurations

Let $M > 0$ and suppose $\omega : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ satisfies $\lim_{R\to\infty} \omega(R) = +\infty$. Then define

$$\mathcal{M}(M,\omega) = \left\{ m : \mathbb{R}^3 \to \mathbb{R}_{\geq 0} \;\middle|\; \|m\|_{L^\infty(\mathbb{R}^3)} \leq M, \right.$$
$$\left. \forall\, R > 0 \;\; \inf_{x\in\mathbb{R}^3} \int_{B_R(x)} m(z)\, \mathrm{d}z \geq \omega(R)R \right\}.$$

Lemma 1 - Uniform Regularity Estimates

Suppose $m \in \mathcal{M}(M,\omega)$, then there exists a unique ground state (u,ϕ) corresponding to m, satisfying (1)-(2) and

$$\|u\|_{C^3(\mathbb{R}^3)} + \|\phi\|_{C^1(\mathbb{R}^3)} \leq C(M), \tag{3}$$
$$\|u\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M), \tag{4}$$
$$\inf_{x\in\mathbb{R}^3} u(x) \geq c_{M,\omega} > 0. \tag{5}$$

Key Ideas of Proof for Lemma 1 - Arguing as in [C/LB/L]

Let $m \in \mathcal{M}(M, \omega)$.

- Let $R > 0$, then define the truncated nuclear distribution $m_R = m\chi_{B_R(0)}$, then find (u_R, ϕ_R) minimising TFW w.r.t m_R.
- Show uniform regularity estimates for u_R, ϕ_R.

$$\|u_R\|_{H^4_{\text{unif}}(\mathbb{R}^3)} + \|\phi_R\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \leq C(M),$$
$$\|u_R\|_{C^3(\mathbb{R}^3)} + \|\phi_R\|_{C^1(\mathbb{R}^3)} \leq C(M).$$

- Pass to the limit $u_R \to u_\infty, \phi_R \to \phi_\infty$ solving

$$-\Delta u_\infty + \tfrac{5}{3} u_\infty^{7/3} - \phi_\infty u_\infty = 0,$$
$$-\Delta \phi_\infty = 4\pi(m - u_\infty^2).$$

  By uniqueness of the TFW equations $(u_\infty, \phi_\infty) = (u, \phi)$.
- Show $\inf_{x \in \mathbb{R}^3} u(x) \geq c_{M,\omega} > 0$, arguing by contradiction.

Convolution Lemma

Lemma - Lieb, Simon (1977)

Suppose $f \in L^p(\mathbb{R}^3), g \in L^q(\mathbb{R}^3)$ such that $p, q > 1, \frac{1}{p} + \frac{1}{q} = 1$, then $f * g$ is a continuous function tending to zero at infinity.

Proof: Since $f \in L^p(\mathbb{R}^3), g \in L^q(\mathbb{R}^3)$ for $p, q > 1$, there exists $f_n, g_n \in C_c^\infty(\mathbb{R}^3)$ such that $f_n \to f, g_n \to g$ in $L^p(\mathbb{R}^3)$ and $L^q(\mathbb{R}^3)$, respectively. By the triangle inequality

$$\|f * g - f_n * g_n\|_{L^\infty(\mathbb{R}^3)} \leq \|f - f_n\|_{L^p(\mathbb{R}^3)}\|g_n\|_{L^q(\mathbb{R}^3)} + \|f\|_{L^p(\mathbb{R}^3)}\|g - g_n\|_{L^q(\mathbb{R}^3)}$$

$f_n * g_n$ form a sequence of continuous compact functions converging uniformly to $f * g$ on $\mathbb{R}^3$, hence $f * g$ is continuous and vanishes at infinity.

Outline of Proof for Lemma 1 - Arguing as in [C/LB/L]

Let $m \in \mathcal{M}(M, \omega)$ and let $R > 0$, then define $m_R = m\chi_{B_R(0)}$. This has a finite, positive charge, The minimisation problem

$$\mathcal{I}^{\mathrm{TFW}}(m_R) = \inf \left\{ E^{\mathrm{TFW}}(v, m_R) \,\middle|\, v \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_R > 0 \right\}$$

yields a unique positive solution $u_R \in H^1(\mathbb{R}^3)$ to

$$-\Delta u_R + \tfrac{5}{3} u_R^{7/3} - \left((m_R - u_R^2) * \tfrac{1}{|\cdot|} \right) u_R = -\theta_R u_R, \qquad (6)$$

where $\theta_R > 0$ is the Lagrange multiplier from the charge constraint. Define

$$\phi_R = \left((m_R - u_R^2) * \tfrac{1}{|\cdot|} \right) - \theta_R,$$

which solves

$$-\Delta \phi_R = 4\pi (m_R - u_R^2)$$

in distribution on $\mathbb{R}^3$.

Outline of Proof for Lemma 1

So (u_R, ϕ_R) solve the finite coupled Schrödinger-Poisson system

$$-\Delta u_R + \frac{5}{3} u_R^{7/3} - \phi_R u_R = 0, \quad (7)$$
$$-\Delta \phi_R = 4\pi(m_R - u_R^2). \quad (8)$$

As $u_R \in H^1(\mathbb{R}^3) \hookrightarrow L^6(\mathbb{R}^3)$, $u_R \in L^p(\mathbb{R}^3)$ for all $p \in [2, 6]$, hence by the decomposition

$$(m_R - u_R^2) * \frac{1}{|\cdot|} = \underbrace{(m_R - u_R^2)}_{\in L^{5/3}(\mathbb{R}^3)} * \underbrace{\left(\frac{1}{|\cdot|}\chi_{B_1(0)}\right)}_{\in L^{5/2}(\mathbb{R}^3)} + \underbrace{(m_R - u_R^2)}_{\in L^{7/5}(\mathbb{R}^3)} * \underbrace{\left(\frac{1}{|\cdot|}\chi_{B_1(0)^c}\right)}_{\in L^{7/2}(\mathbb{R}^3)},$$

so $\phi_R = \left((m_R - u_R^2) * \frac{1}{|\cdot|}\right) - \theta_R \in L^\infty(\mathbb{R}^3)$ is continuous and converges to $-\theta_R < 0$ at infinity.

Outline of Proof for Lemma 1

As $u_R \geq 0$,

$$-\Delta u_R + u_R \leq (1+\phi_R)u_R.$$

Since $(1+\phi_R)u_R \in L^2(\mathbb{R}^3)$, by Lax-Milgram there exists unique $g \in H^1(\mathbb{R}^3)$ satisfying

$$-\Delta g + g = (1+\phi_R)u_R.$$

In fact, using the Green's function $\frac{e^{-|x|}}{|x|} \in L^2(\mathbb{R}^3)$,

$$g = \frac{e^{-|x|}}{|x|} * (1+\phi_R)u_R$$

satisfies $\|g\|_{L^\infty(\mathbb{R}^3)} \leq C(1+\|\phi_R\|_{L^\infty(\mathbb{R}^3)})\|u_R\|_{L^2(\mathbb{R}^3)}$.

By the maximum principle $u_R \leq g \leq C(1+\|\phi_R\|_{L^\infty(\mathbb{R}^3)})\|u_R\|_{L^2(\mathbb{R}^3)}$ and u_R vanishes at infinity.

Outline of Proof for Lemma 1

So far, we have shown $u_R, \phi_R \in L^\infty(\mathbb{R}^3)$ are continuous and shown decay properties at infinity. However, we have yet to show uniform $L^\infty(\mathbb{R}^3)$ estimates.

Use the Sovolej estimate [Sovolej (1990)], there exists a universal constant $C_S > 0$ such that

$$\frac{10}{9} u_R^{4/3} \leq \phi_R + C_S, \tag{9}$$
$$0 < \theta_R \leq C_S.$$

Since $u_R \geq 0$, this gives the lower bound

$$\phi_R \geq -C_S,$$

so it remains to show $\|\phi_R^+\|_{L^\infty(\mathbb{R}^3)} \leq C(M)$, then it would follow that

$$\|u_R\|_{L^\infty(\mathbb{R}^3)}^{4/3} \leq C_S + \|\phi_R\|_{L^\infty(\mathbb{R}^3)} \leq C(M).$$

Outline of Proof for Lemma 1

Suppose for now that the estimate holds

$$\|u_R\|_{L^\infty(\mathbb{R}^3)}^{4/3} \leq C_S + \|\phi_R\|_{L^\infty(\mathbb{R}^3)} \leq C(M).$$

Applying standard interior elliptic regularity results we obtain

$$\|u_R\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_R\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M).$$

Using Schauder estimates of the form [Jost (2002)]

$$\|\phi_R\|_{C^{1,\alpha}(B_1(x))} \leq C\left(\|m_R - u_R^2\|_{L^4(B_2(x))} + \|\phi_R\|_{L^2(B_2(x))}\right),$$

we deduce

$$\|u_R\|_{C^3(\mathbb{R}^3)} + \|\phi_R\|_{C^1(\mathbb{R}^3)} \leq C(M).$$

Then by passing to the limit and using uniqueness, we obtain the desired estimates for the ground state (u, ϕ).

Outline of Proof for Lemma 1

Suppose w.l.o.g that $\phi_R^+(0) = \|\phi_R^+\|_{L^\infty(\mathbb{R}^3)}$.
Let $\varphi \in C_c^\infty(B_1(0))$ satisfy $0 \le \varphi \le 1$, $\int_{\mathbb{R}^3} \varphi^2 = 1$.

Key ideas: Define $\phi_R^* = \phi_R * \varphi^2$, which satisfies

$$-\Delta \phi_R^* + (\phi_R^* - C)_+^{3/2} \le C_0 M.$$

By the maximum principle, $\phi_R^* \le C(1 + M^{2/3})$. Then one can show ϕ_R^+ satisfies

$$-\Delta \phi_R^+ \le C_0 M \quad \text{in } B_t(0),$$
$$\fint_{S_t(0)} \phi_R^+ \, \mathrm{d}\sigma_t \le C(1 + M^{2/3}).$$

By constructing g solving

$$-\Delta g = C_0 M \quad \text{in } B_t(0),$$
$$g = \phi_R^+ \quad \text{on } S_t(0),$$

by the maximum principle $\phi_R^+ \le g$.

Outline of Proof for Lemma 1

In particular, by the mean value property for harmonic functions

$$\phi_R^+(0) \leq g(0) = \fint_{S_t(0)} \phi_R^+ \, \mathrm{d}\sigma_t + CM \leq C(1+M),$$

hence

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

and the following estimate holds

$$\|u_R\|_{L^\infty(\mathbb{R}^3)}^{4/3} \leq C_S + \|\phi_R\|_{L^\infty(\mathbb{R}^3)} \leq C(M).$$

Pointwise Stability Estimates

Theorem 1

Suppose that for $i = 1, 2$ $m_i \in \mathcal{M}(M, \omega)$, then the corresponding ground states (u_i, ϕ_i) solving

$$\begin{array}{ll} -\Delta u_1 + \frac{5}{3} u_1^{7/3} - \phi_1 u_1 = 0, & -\Delta u_2 + \frac{5}{3} u_2^{7/3} - \phi_2 u_2 = 0, \\ -\Delta \phi_1 = 4\pi(m_1 - u_1^2), & -\Delta \phi_2 = 4\pi(m_2 - u_2^2), \end{array}$$

then there exists $C(M, \omega), \gamma(M, \omega) > 0$ such that for all $y \in \mathbb{R}^3$

$$|(u_1 - u_2)(y)| + |(\phi_1 - \phi_2)y| \leq C \left(\int_{\mathbb{R}^3} |(m_1 - m_2)(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x \right)^{1/2} \tag{10}$$

Application I

Corollary

Let $m_1, m_2 \in \mathcal{M}(M, \omega)$.

- (Local estimates) Suppose $m_1 - m_2$ has support in $B_R(0)$. Then

$$|(u_1 - u_2)(y)| + |(\phi_1 - \phi_2)(y)| \leq C(R)e^{-\gamma|y|}.$$

- (Decay estimates) Suppose that

$$|(m_1 - m_2)(x)| \leq C(1 + |x|)^{-r},$$

  for some $r > 0$, then

$$|(u_1 - u_2)(y)| + |(\phi_1 - \phi_2)(y)| \leq C(r)(1 + |y|)^{-r}.$$

- (Global estimates) Suppose $m_1 - m_2 \in L^2(\mathbb{R}^3)$, then

$$\|u_1 - u_2\|_{H^4(\mathbb{R}^3)} + \|\phi_1 - \phi_2\|_{H^2(\mathbb{R}^3)} \leq C\|m_1 - m_2\|_{L^2(\mathbb{R}^3)}.$$

Application II - Neutrality

Theorem 2 - Neutrality of Local Defects

Let $m_1, m_2 \in \mathcal{M}_0(M, \omega)$ and suppose that $m_1 - m_2$ has support in $B_{R'}(0)$ for some $R' > 0$. Then

$$\int_{\mathbb{R}^3} (m_1 - u_1^2 - m_2 + u_2^2) = 0,$$

hence local defects are neutral in the TFW model.

Application II - Neutrality

Proof: Let $\varphi \in C_c^\infty(B_2(0))$ such that $0 \leq \varphi \leq 1$ and $\varphi = 1$ on $B_1(0)$ and for $R > 0$ define, $\varphi_R = \varphi(\cdot/R)$. Recall

$$-\Delta(\phi_1 - \phi_2) = 4\pi(m_1 - m_2 - u_1^2 + u_2^2),$$

so testing this with φ_R gives

$$-\int_{B_{2R}(0)} \Delta(\phi_1 - \phi_2)\varphi_R = 4\pi \int_{B_{2R}(0)} (m_1 - u_1^2 - m_2 + u_2^2)\varphi_R.$$

Using IBP, the left-hand side is

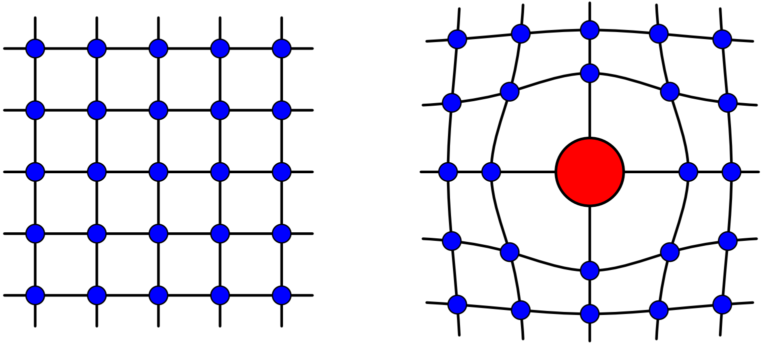
$$-\int_{B_{2R}(0)} (\phi_1 - \phi_2)\Delta\varphi_R = -\frac{1}{R^2}\int_{B_{2R}(0)\setminus B_R(0)} (\phi_1 - \phi_2)(\Delta\varphi)(\cdot/R),$$

This gives

$$\left| \int_{B_{2R}(0)} (m_1 - u_1^2 - m_2 + u_2^2)\varphi_R \right| \leq \frac{C}{R^2}\int_{B_{2R}(0)\setminus B_R(0)} |(\phi_1 - \phi_2)(x)| \, \mathrm{d}x$$

$$\leq \frac{C}{R^2}\int_{B_{2R}(0)\setminus B_R(0)} e^{-\gamma|x|} \, \mathrm{d}x = \frac{C}{R^2}\int_R^{2R} r^2 e^{-\gamma r} \, \mathrm{d}r = Ce^{-\gamma R}.$$

Outlook



$$\mathcal{I} = \inf\{\, \mathcal{E}(U_\Lambda) \mid U_\Lambda \in \mathcal{U}^{1,2} \,\}, \quad \mathcal{I}^{d} = \inf\{\, \mathcal{E}^{d}(U_\Lambda) \mid U_\Lambda \in \mathcal{U}^{1,2} \,\}.$$

The TFW energy minimisation problems $\mathcal{I}, \mathcal{I}^{d}$ are well-defined.

Outlook

- Construction of TFW site energy.
- Approximating the global minimisation problem by a finite problem.
- Numerical simulations.
- Dislocations.

Thank you for your attention!