Local Defects in the Thomas-Fermi-von Weizsäcker Theory of Crystals

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Multiscale Models of Crystal Defects, Banff

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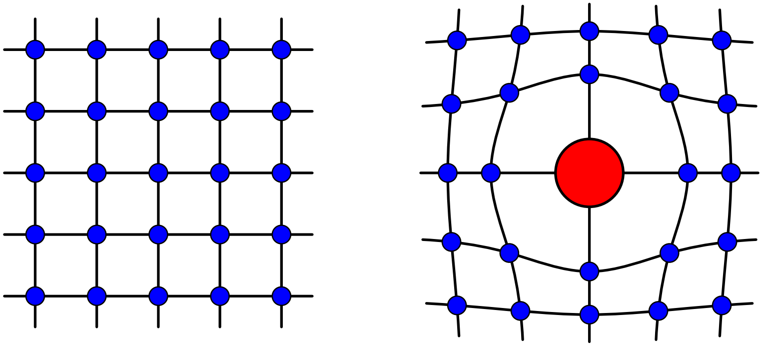
Motivation



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

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
- Exponential Estimates
- Applications of the Exponential Estimates
- Renormalising the Energy Differences
- 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

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

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:

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

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

$$-\Delta u + \frac{5}{3}u^{7/3} - \phi u = 0, \tag{2}$$

$$-\Delta \phi = 4\pi(m - u^2), \tag{3}$$

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

Lattice Displacements

Let $\Lambda = \mathbb{Z}^3$ and e_1, e_2, e_3 denote the standard normal basis of $\mathbb{R}^3$.

$$\mathcal{U} = \mathcal{U}^{1,2} = \{U_\Lambda : \Lambda \to \mathbb{R}^3 \mid \|\nabla U_\Lambda\|_{\ell^2(\Lambda)} < \infty\},$$

$$\|\nabla U_\Lambda\|_{\ell^2(\Lambda)} = \left(\sum_{l \in \Lambda} \sum_{i=1}^{3} |U_\Lambda(l + e_i) - U_\Lambda(l)|^2 \right)^{1/2}$$

$$\sim \|\nabla U_\Lambda\|_\gamma = \left(\sum_{l \in \Lambda} \sum_{\rho \in \Lambda \setminus \{0\}} e^{-\gamma|\rho|} |U_\Lambda(l + \rho) - U_\Lambda(l)|^2 \right)^{1/2}.$$

Useful embeddings,

$$\mathcal{U}^{1,2} \hookrightarrow \ell^6(\Lambda) \hookrightarrow \ell^\infty(\Lambda),$$

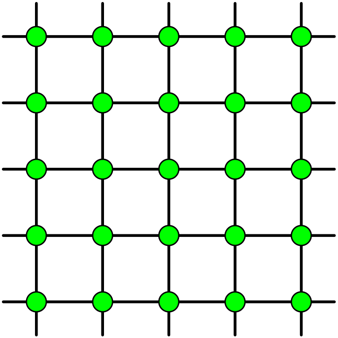
by the Gagliardo-Nirenberg-Sobolev embedding theorem.

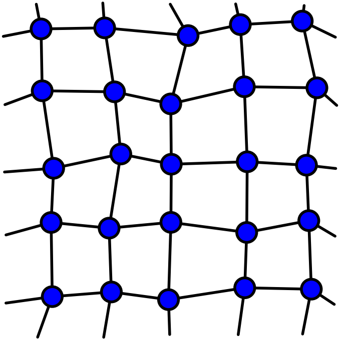
Also, define

$$\mathcal{U}^c = \{ V_\Lambda \in \mathcal{U}^{1,2} \mid V_\Lambda \text{ has compact support}\}.$$

Nuclear Configurations

Let $\eta \in C_c^2(B_{1/4}(0))$ be non-negative and radial.





$$m_{per}(x) = \sum_{l \in \Lambda} \eta(x - l), \qquad m_U(x) = \sum_{l \in \Lambda} \eta(x - l - U_\Lambda(l)),$$

$$-\Delta u_{per} + \tfrac{5}{3} u_{per}^{7/3} - \phi_{per} u_{per} = 0, \qquad -\Delta u_U + \tfrac{5}{3} u_U^{7/3} - \phi_U u_U = 0,$$

$$-\Delta \phi_{per} = 4\pi(m_{per} - u_{per}^2), \qquad -\Delta \phi_U = 4\pi(m_U - u_U^2).$$

Homogeneous Energy Difference

For $U_\Lambda \in \mathcal{U}^{1,2}$, define

$$\mathcal{E}(U_\Lambda) = E^{TFW}(u_U, m_U) - E^{TFW}(u_{per}, m_{per})$$
$$= \int |\nabla u_U|^2 + \int u_U^{10/3} + \frac{1}{2}\int \phi_U(m_U - u_U^2)$$
$$- \int |\nabla u_{per}|^2 - \int u_{per}^{10/3} - \frac{1}{2}\int \phi_{per}(m_{per} - u_{per}^2).$$

Since $m_{per}, m_U \in C^2(\mathbb{R}^3)$, by elliptic regularity

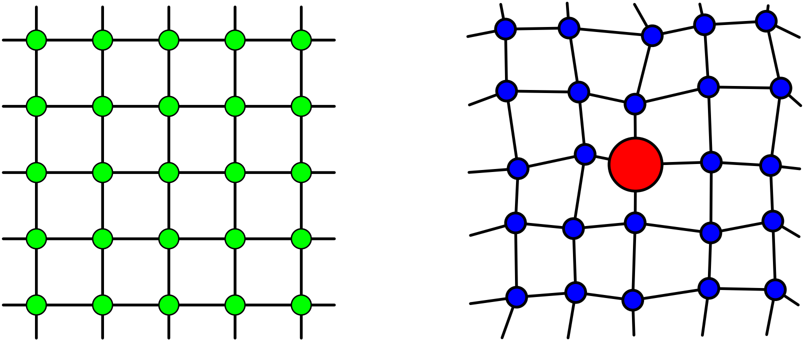
$$u_U, u_{per}, \phi_U, \phi_{per} \in W^{4,\infty}(\mathbb{R}^3).$$

Direct estimates give

$$|\mathcal{E}(U_\Lambda)| \leq C(\|u_U - u_{per}\|_{W^{1,1}(\mathbb{R}^3)} + \|\phi_U - \phi_{per}\|_{L^1(\mathbb{R}^3)} + \|m_U - m_{per}\|_{L^1(\mathbb{R}^3)}). \quad (4)$$

Nuclear Configurations

Let $\rho_{def}^{nuc} \in C_c^2(\mathbb{R}^3)$ represent the density of a defect.



$$m_{per}(x) = \sum_{l \in \Lambda} \eta(x - l), \qquad m_{U,d}(x) = m_U(x) + \rho_{def}^{nuc}(x - U_\Lambda(0)) \geq 0,$$

$$-\Delta u_{per} + \tfrac{5}{3} u_{per}^{7/3} - \phi_{per} u_{per} = 0, \qquad -\Delta u_{U,d} + \tfrac{5}{3} u_{U,d}^{7/3} - \phi_{U,d} u_{U,d} = 0,$$
$$-\Delta \phi_{per} = 4\pi(m_{per} - u_{per}^2), \qquad -\Delta \phi_{U,d} = 4\pi(m_{U,d} - u_{U,d}^2).$$

Defective Energy Difference

For $U_\Lambda \in \mathcal{U}^{1,2}$, define

$$\begin{aligned}
\mathcal{E}^{d}(U_\Lambda) &= E^{TFW}(u_{U,d}, m_{U,d}) - E^{TFW}(u_{per}, m_{per}) \\
&= \int |\nabla u_{U,d}|^2 + \int u_{U,d}^{10/3} + \frac{1}{2}\int \phi_{U,d}(m_{U,d} - u_{U,d}^2) \\
&\quad - \int |\nabla u_{per}|^2 - \int u_{per}^{10/3} - \frac{1}{2}\int \phi_{per}(m_{per} - u_{per}^2).
\end{aligned}$$

Similarly,

$$\begin{aligned}
|\mathcal{E}^{d}(U_\Lambda)| \leq C(&\|u_{U,d} - u_{per}\|_{W^{1,1}(\mathbb{R}^3)} + \|\phi_{U,d} - \phi_{per}\|_{L^1(\mathbb{R}^3)} \\
&+ \|m_{U,d} - m_{per}\|_{L^1(\mathbb{R}^3)}).
\end{aligned}$$

Translational Invariance

For any $c \in \mathbb{R}^3$, $\quad m_{U+c} = m_U(\cdot - c), \quad m_{U+c,d} = m_{U,d}(\cdot - c),$

$$\implies \mathcal{E}(U_\Lambda + c) = \mathcal{E}(U_\Lambda), \quad \mathcal{E}^{d}(U_\Lambda + c) = \mathcal{E}^{d}(U_\Lambda). \tag{5}$$

Energy Differences

Questions:

1. For $U_\Lambda \in \mathcal{U}^{1,2}$, how do we compare (u_U, ϕ_U) and (u_{per}, ϕ_{per})?
2. Are $\mathcal{E}(U_\Lambda), \mathcal{E}^{d}(U_\Lambda)$ well-defined for all $U_\Lambda \in \mathcal{U}^{1,2}$?
3. Regularity of $\mathcal{E}, \mathcal{E}^{d}$?
4. Do minimisers decay?

Strategy:

- For 1, show exponential estimates.
- Answer 2 and 3 for $U_\Lambda \in \mathcal{U}^c$.
- Utilise lattice symmetries when $U_\Lambda = 0$
  and translational invariance for all $U_\Lambda \in \mathcal{U}^{1,2}$.
- Find a suitable renormalisation, use the density of $\mathcal{U}^c$ in $\mathcal{U}^{1,2}$.
- Answer 2 and 3 for $U_\Lambda \in \mathcal{U}^{1,2}$.

Exponential Estimates

Theorem 1

Suppose that m_1, m_2 are nuclear arrangements satisfying (H1), (H2) and $m_2 - m_1 = R_{nuc} \in W^{1,\infty}(\mathbb{R}^3)$. Then there exist unique solutions to the following systems

$$\begin{array}{ll} -\Delta u_1 + \frac{5}{3} u_1^{7/3} - \phi_1 u_1 = 0, & -\Delta u_2 + \frac{5}{3} u_2^{7/3} - \phi_2 u_2 = 0, \\ -\Delta \phi_1 = 4\pi(m_1 - u_1^2), & -\Delta \phi_2 = 4\pi(m_1 - u_2^2) + R_{nuc}, \end{array} \tag{6}$$

with $u_1, u_2, \phi_1, \phi_2 \in W^{3,\infty}(\mathbb{R}^3)$.
Then there exists $C, \widetilde{\gamma} > 0$ such that for all $0 < \gamma \leq \widetilde{\gamma}$ and all $y \in \mathbb{R}^3$

$$\int_{\mathbb{R}^3} \sum_{|\alpha| \leq 3} \left(|\partial^\alpha (u_1 - u_2)(x)|^2 + |\partial^\alpha (\phi_1 - \phi_2)(x)|^2 \right) e^{-2\gamma|x-y|} \, dx$$
$$\leq C \int_{\mathbb{R}^3} \sum_{|\beta| \leq 1} |\partial^\beta R_{nuc}(x)|^2 e^{-2\gamma|x-y|} \, dx. \tag{7}$$

Corollary 2

Suppose the conditions for Theorem 1 are satisfied and in addition $R_{nuc} \in H^1(\mathbb{R}^3)$, then

$$\|u_1 - u_2\|_{H^3(\mathbb{R}^3)} + \|\phi_1 - \phi_2\|_{H^3(\mathbb{R}^3)} \leq C\|R_{nuc}\|_{H^1(\mathbb{R}^3)}. \tag{8}$$

Remark: The constants C from Theorem 1 and Corollary 2 depend on

$$C = C\big(\inf(u_1+u_2)^{-1}, \max\{\|u_1\|_{W^{1,\infty}}, \|u_2\|_{W^{1,\infty}}\}, \max\{\|\phi_1\|_{W^{1,\infty}}, \|\phi_2\|_{W^{1,\infty}}\}\big).$$

Sketch Proof of Theorem 1

Define $w = u_1 - u_2, \psi = \phi_1 - \phi_2$.

Key steps:

1. Initial estimates: fix $\xi \in H^1(\mathbb{R}^3)$, then

$$\int_{\mathbb{R}^3} |\nabla w|^2 \xi^2 + \int_{\mathbb{R}^3} w^2 \xi^2 + \int_{\mathbb{R}^3} |\nabla \psi|^2 \xi^2 \leq C \left(\int_{\mathbb{R}^3} R_{nuc} \psi \xi^2 + \int_{\mathbb{R}^3} \left(w^2 + \psi^2\right) |\nabla \xi|^2 \right). \quad (9)$$

2. Higher order estimates:

$$\int_{\mathbb{R}^3} \psi^2 \xi^2 + \int_{\mathbb{R}^3} \sum_{2 \leq |\alpha| \leq 3} \left(|\partial^\alpha w|^2 + |\partial^\alpha \psi|^2 \right) \xi^2 \leq C \left(\int_{\mathbb{R}^3} \sum_{|\beta| \leq 1} |\partial^\beta R_{nuc}|^2 \xi^2 + \int_{\mathbb{R}^3} \left(w^2 + \psi^2\right) |\nabla \xi|^2 \right). \quad (10)$$

Proof of Theorem 1

3. Combine (9) and (10)

$$\int_{\mathbb{R}^3} \sum_{|\alpha|\le 3} \left(|\partial^\alpha w|^2 + |\partial^\alpha \psi|^2\right)\xi^2$$

$$\le C^* \left(\int_{\mathbb{R}^3} \sum_{|\beta|\le 1} |\partial^\beta R_{nuc}|^2 \xi^2 + \int_{\mathbb{R}^3} \left(w^2 + \psi^2\right) |\nabla \xi|^2 \right). \tag{11}$$

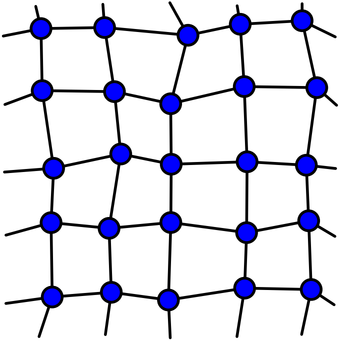
Let $y \in \mathbb{R}^3$ and $0 < \gamma \le \widetilde{\gamma} = \frac{1}{\sqrt{2C^*}}$, then choose

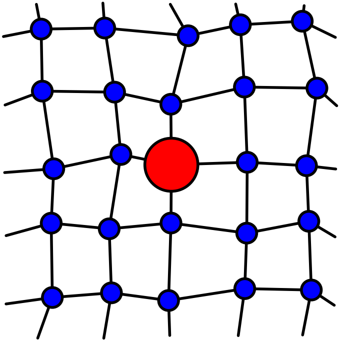
$$\xi(x) = e^{-\gamma|x-y|} \implies |\nabla \xi(x)|^2 \le \frac{1}{2C^*}\xi^2(x).$$

Finally, this gives

$$\int_{\mathbb{R}^3} \sum_{|\alpha|\le 3} \left(|\partial^\alpha w|^2 + |\partial^\alpha \psi|^2\right)\xi^2 \le C \int_{\mathbb{R}^3} \sum_{|\beta|\le 1} |\partial^\beta R_{nuc}|^2 \xi^2.$$

Let $U_\Lambda \in \mathcal{U}^{1,2}$, consider





$$-\Delta u_U + \tfrac{5}{3}u_U^{7/3} - \phi_U u_U = 0, \qquad -\Delta u_{U,d} + \tfrac{5}{3}u_{U,d}^{7/3} - \phi_{U,d} u_{U,d} = 0,$$
$$-\Delta \phi_U = 4\pi(m_U - u_U^2), \qquad -\Delta \phi_{U,d} = 4\pi(m_U - u_{U,d}^2) + \rho_{def}^{nuc},$$

$$R_m = \rho_{def}^{nuc} \in C_c^2(B_R(U_\Lambda(0))).$$

Application I.I - Local Defects

Lemma (Application I.I)

Let $U_\Lambda \in \mathcal{U}^{1,2}$*, then there exists* $C(U_\Lambda, \rho_{def}^{nuc}), \gamma(U_\Lambda, \rho_{def}^{nuc}) > 0$ *such that*

$$\begin{matrix} |(u_{U,d} - u_U)(y)| + |\nabla(u_{U,d} - u_U)(y)| \\ |(\phi_{U,d} - \phi_U)(y)| + |\nabla(\phi_{U,d} - \phi_U)(y)| \end{matrix} \leq Ce^{-\gamma|y-U_\Lambda(0)|}. \qquad (12)$$

Proof: Let $w = u_V - u_{per}, \psi = \phi_V - \phi_{per}$.

Applying Theorem 1 gives

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

$$\leq C \int_{B_{R'}(z)} \left(|R_m(x)|^2 + |\nabla R_m(x)|^2 \right) e^{-2\gamma|x-y|} \, \mathrm{d}x$$

$$\leq C \, \|R_m\|^2_{H^1(B_{R'}(U_\Lambda(0)))} \, e^{-2\gamma|y-z|}.$$

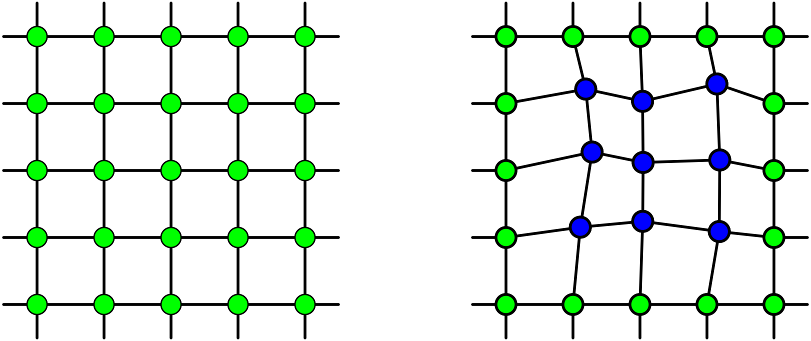
Application I.I - Local Defects

Idea: Restrict the integral to $B_1(y)$ and use the embedding $H^3(B_1(y)) \hookrightarrow C^{1,\alpha}(B_1(y))$.

$$
\begin{aligned}
&\left(|w(y)|^2 + |\nabla w(y)|^2 + |\psi(y)|^2 + |\nabla \psi(y)|^2\right) \\
&\leq C \left(\|w\|^2_{C^{1,\alpha}(B_1(y))} + \|\psi\|^2_{C^{1,\alpha}(B_1(y))} \right) \\
&\leq C \left(\|w\|^2_{H^3(B_1(y))} + \|\psi\|^2_{H^3(B_1(y))} \right) \\
&\leq C e^{2\gamma} \int_{B_1(y)} \sum_{|\alpha| \leq 3} \left(|\partial^\alpha w(x)|^2 + |\partial^\alpha \psi(x)|^2 \right) e^{-2\gamma|x-y|} \, \mathrm{d}x \\
&\leq C \int_{\mathbb{R}^3} \sum_{|\alpha| \leq 3} \left(|\partial^\alpha w(x)|^2 + |\partial^\alpha \psi(x)|^2 \right) e^{-2\gamma|x-y|} \, \mathrm{d}x \\
&\leq C \, \|R_m\|^2_{H^1(B_{R'}(U_\Lambda(0)))} \, e^{-2\gamma|y-U_\Lambda(0)|}.
\end{aligned}
$$

Application I.II - Compact Displacements

Let $V_\Lambda \in \mathcal{U}^c$ with $\mathrm{spt}(V_\Lambda) \subset B_R(z)$.



$$-\Delta u_{per} + \tfrac{5}{3} u_{per}^{7/3} - \phi_{per} u_{per} = 0, \qquad -\Delta u_V + \tfrac{5}{3} u_V^{7/3} - \phi_V u_V = 0,$$
$$-\Delta \phi_{per} = 4\pi(m_{per} - u_{per}^2), \qquad -\Delta \phi_V = 4\pi(m_V - u_V^2),$$

$$R_m = m_V - m_{per} \in C_c^2(B_{R'}(z)).$$

Application I.II - Compact Displacements

Lemma (Application I.II)

Let $V_\Lambda \in \mathcal{U}^c$ *with* $\operatorname{spt}(V_\Lambda) \subset B_R(z)$. *Then there exists* $C(V_\Lambda), \gamma(V_\Lambda) > 0$ *such that*

$$\left.\begin{array}{r} |(u_V - u_{per})(y)| + |\nabla(u_V - u_{per})(y)| \\ |(\phi_V - \phi_{per})(y)| + |\nabla(\phi_V - \phi_{per})(y)| \end{array}\right. \leq Ce^{-\gamma|y-z|}. \tag{13}$$

Proof: This follows immediately from the proof of Application I.I. □

Energy Differences for Compact Displacments

Proposition 3

$\mathcal{E}, \mathcal{E}^{d} : \mathcal{U}^c \to \mathbb{R}$ are well-defined.

Proof: Let $V_\Lambda \in \mathcal{U}^c$ with $\mathrm{spt}(V_\Lambda) \subset B_R(z)$, then by Applications I.I and I.II,

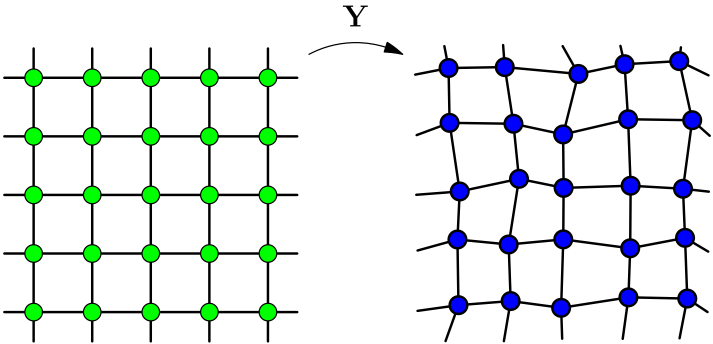
$$\begin{aligned} m_V - m_{per}, m_{V,d} - m_{per} &\in C_c^2(\mathbb{R}^3) \subset L^1(\mathbb{R}^3), \\ |\nabla(u_V - u_{per})|, |u_V - u_{per}|, |\phi_V - \phi_{per}| &\leq Ce^{-\gamma|\cdot - z|} \in L^1(\mathbb{R}^3), \\ |\nabla(u_{V,d} - u_{per})|, |u_{V,d} - u_{per}|, |\phi_{V,d} - \phi_{per}| & \\ &\leq C(e^{-\gamma|\cdot - z|} + e^{-\gamma|\cdot - U_\Lambda(0)|}) \in L^1(\mathbb{R}^3), \end{aligned}$$

hence by direct estimates (4),

$$|\mathcal{E}(V_\Lambda)| < \infty, \qquad |\mathcal{E}^{d}(V_\Lambda)| < \infty.$$

Application II - Change of Variables Estimates

Let $U_\Lambda \in \mathcal{U}^{1,2}$, now consider



$$-\Delta u_{per} + \tfrac{5}{3} u_{per}^{7/3} - \phi_{per} u_{per} = 0, \qquad -\Delta u_U + \tfrac{5}{3} u_U^{7/3} - \phi_U u_U = 0,$$
$$-\Delta \phi_{per} = 4\pi(m_{per} - u_{per}^2), \qquad -\Delta \phi_U = 4\pi(m_U - u_U^2).$$

Application II - Change of Variables Estimates

We can not estimate $u_U - u_{per}$ directly, instead we use (u_{per}, ϕ_{per}) and U_Λ to construct predictor variables $(\widetilde{u}_U, \widetilde{\phi}_U)$.

Application II

Let $U_\Lambda \in \mathcal{U}^{1,2}$, then there exists $(\widetilde{u}_U, \widetilde{\phi}_U) \in W^{4,\infty}(\mathbb{R}^3)$ satisfying

$$\|u_U - \widetilde{u}_U\|_{H^3(\mathbb{R}^3)} + \|\phi_U - \widetilde{\phi}_U\|_{H^3(\mathbb{R}^3)} \leq C\|\nabla U_\Lambda\|_{\ell^2(\Lambda)}. \tag{14}$$

Proof: Let $U_\Lambda \in \mathcal{U}^{1,2}$. We interpolate U_Λ to $\mathbb{R}^3$ to find $\mathbf{U}, \mathbf{Y} \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$, satisfying:

$$\begin{aligned} &\mathbf{Y} \text{ is invertible}, \\ &\mathbf{Y}(x) = x + \mathbf{U}(x), \\ &\|\nabla \mathbf{U}\|_{L^2(\mathbb{R}^3)} + \|\nabla^2 \mathbf{U}\|_{L^2(\mathbb{R}^3)} \leq C\|\nabla U_\Lambda\|_{\ell^2(\Lambda)}. \end{aligned} \tag{15}$$

The predictor variables are defined by

$$\widetilde{u}_U = u_{per} \circ \mathbf{Y}^{-1}, \qquad \widetilde{\phi}_U = \phi_{per} \circ \mathbf{Y}^{-1}.$$

Application II - General estimates

Also,

$$m_{per} \circ \mathbf{Y}^{-1} = m_U + R_{nuc},$$

where $R_{nuc} \in C_c^\infty(B_R(0))$. The predictors $(\widetilde{u}_U, \widetilde{\phi}_U)$ satisfy

$$-\Delta \widetilde{u}_U + \tfrac{5}{3}\widetilde{u}_U^{7/3} - \widetilde{\phi}_U \widetilde{u}_U = R_1, \qquad -\Delta u_U + \tfrac{5}{3} u_U^{7/3} - \phi_U u_U = 0,$$
$$-\Delta \widetilde{\phi}_U = 4\pi(m_U - \widetilde{u}_U^2) + R_2 + R_{nuc}, \qquad -\Delta \phi_U = 4\pi(m_U - u_U^2).$$

The residual terms $R_1, R_2, R_{\mathrm{nuc}}$ satisfy

$$\sum_{|\beta|\le 1} \Big(|\partial^\beta R_1(x)| + |\partial^\beta R_2(x)| + |\partial^\beta R_{nuc}(x)| \Big)$$
$$\le C\big(|\nabla \mathbf{U}(x)| + |\nabla^2 \mathbf{U}(x)|\big) \in L^2(\mathbb{R}^3).$$

By Corollary 1, we have

$$\|u_U - \widetilde{u}_U\|_{H^3(\mathbb{R}^3)} + \|\phi_U - \widetilde{\phi}_U\|_{H^3(\mathbb{R}^3)}$$
$$\le C\|\nabla \mathbf{U}\|_{L^2(\mathbb{R}^3)} + \|\nabla^2 \mathbf{U}\|_{L^2(\mathbb{R}^3)} \le C\|\nabla U_\Lambda\|_{\ell^2(\Lambda)}. \quad \square$$

Application III - Decay estimates

Application III

Let $U_\Lambda \in \mathcal{U}^{1,2}$ and suppose

$$|\nabla U_\Lambda(l)| \leq C(1+|l|)^{-j}$$

Then

$$\begin{matrix} |(u_U - \widetilde{u}_U)(y)| + |\nabla(u_U - \widetilde{u}_U)(y)| \\ |(\phi_U - \widetilde{\phi}_U)(y)| + |\nabla(\phi_U - \widetilde{\phi}_U)(y)| \end{matrix} \leq C(1+|y|)^{-j}. \tag{16}$$

Proof:

$$\begin{aligned} & |\nabla U_\Lambda(l)| \leq C(1+|l|)^{-j} \\ \implies & |\nabla \mathbf{U}(x)| + |\nabla^2 \mathbf{U}(x)| \leq C(1+|x|)^{-j}. \end{aligned}$$

Application III - Decay estimates

Using Theorem 1,

$$\begin{aligned}
&\int_{\mathbb{R}^3} \sum_{|\alpha|\leq 3} \left(|\partial^\alpha (u_U - \widetilde{u}_U)(x)|^2 + |\partial^\alpha (\phi_U - \widetilde{\phi}_U)(x)|^2 \right) e^{-2\gamma|x-y|} \, \mathrm{d}x \\
&\qquad \leq C \int_{\mathbb{R}^3} \left(|\nabla \mathbf{U}(x)|^2 + |\nabla^2 \mathbf{U}(x)|^2 \right) e^{-2\gamma|x-y|} \, \mathrm{d}x \\
&\qquad \leq C \int_{\mathbb{R}^3} (1+|x|)^{-2j} \, e^{-2\gamma|x-y|} \, \mathrm{d}x \\
&\qquad \leq C \, (1+|y|)^{-2j}.
\end{aligned}$$

Arguing as in Application I.I gives

$$\begin{matrix} |(u_U - \widetilde{u}_U)(x)| + |\nabla (u_U - \widetilde{u}_U)(x)| \\ |(\phi_U - \widetilde{\phi}_U)(x)| + |\nabla (\phi_U - \widetilde{\phi}_U)(x)| \end{matrix} \leq C(1+|x|)^{-j}. \quad \square$$

Variations of the Energy Difference

For $U_\Lambda \in \mathcal{U}^{1,2}$, $V_\Lambda, V_1, V_2 \in \mathcal{U}^c$

$$\langle \delta\mathcal{E}(U_\Lambda), V_\Lambda \rangle \text{ is well-defined,}$$

$$\langle \delta^2\mathcal{E}(U_\Lambda)V_1, V_2 \rangle = \sum_{i,j\in\Lambda} V_1(i)^T H_{i,j}(U_\Lambda) V_2(j),$$

where for $i \neq j$

$$H_{i,j}(U_\Lambda) = -\int \Psi_{U,i}(x) \cdot \nabla\eta(x - j - U_\Lambda(j))\,\mathrm{d}x,$$

$$|H_{i,j}(U_\Lambda)| \le C\, e^{-\gamma|i+U_\Lambda(i)-i-U_\Lambda(j)|}.$$

Translational Invariance:

$$\sum_{i\in\Lambda} H_{i,j}(U_\Lambda) = \sum_{j\in\Lambda} H_{i,j}(U_\Lambda) = 0.$$

Consequently

$$\langle \delta^2\mathcal{E}(U_\Lambda)V_1, V_2 \rangle = \sum_{i,j\in\Lambda} V_1(i)^T H_{i,j}(U_\Lambda) \left(V_2(j) - V_2(i)\right).$$

Renormalisation Sketch (*)

Lattice symmetries: for $U_\Lambda = 0, V_\Lambda, V_1, V_2 \in \mathcal{U}^{1,2}$

$$\mathcal{E}(0) = 0, \quad \langle \delta\mathcal{E}(0), V_\Lambda \rangle = 0,$$
$$|\langle \delta^2\mathcal{E}(0) V_1, V_2 \rangle| \le C \|\nabla V_1\|_{\ell^2(\Lambda)} \|\nabla V_2\|_{\ell^2(\Lambda)},$$

using the lattice Fourier transform.

Changes of Variables Estimate:

$$\begin{aligned}
|H_{i,j}(U_\Lambda) - H_{i,j}(0)| = | \int \Psi_{U,i}(x) \cdot \nabla\eta(x - j - U_\Lambda(j)) \, \mathrm{d}x \\
- \int \Psi_{0,i}(x) \cdot \nabla\eta(x - j) \, \mathrm{d}x| \\
\approx \left| \int (\Psi_{U,i}(x) - \widetilde{\Psi}_{U,i}(x)) \cdot \nabla\eta(x - j - U_\Lambda(j)) \, \mathrm{d}x \right| \\
\approx F_i(U_\Lambda) e^{-\gamma|x-i|}.
\end{aligned}$$

Renormalisation Sketch (*)

$F(U_\Lambda) : \Lambda \to \mathbb{R}$ is approximately

$$F_i(U_\Lambda) \approx \left(\int |\nabla \mathbf{U}(x)|^2 e^{-2\gamma|x-i|} \, \mathrm{d}x \right)^{1/2},$$

$$\|F(U_\Lambda)\|_{\ell^2(\Lambda)} \leq C\|\nabla U_\Lambda\|_{\ell^2(\Lambda)}.$$

Renormalisation Sketch (*)

For $V_1, V_2 \in \mathcal{U}^c$

$$
\begin{aligned}
&|\langle \big(\delta^2\mathcal{E}(U_\Lambda) - \delta^2\mathcal{E}(0)\big) V_1, V_2\rangle| \\
&\qquad \le \sum_{i,j\in\Lambda} |V_1(i)| F_i(U_\Lambda) e^{-\gamma|i-j|} |V_2(j) - V_2(i)| \\
&\qquad \le \sum_{l\in\Lambda} \sum_{\rho\in\Lambda\setminus\{0\}} \left(|V_1(l)| F_l(U_\Lambda) e^{-\gamma/2|\rho|}\right) \left(e^{-\gamma/2|\rho|} |D_\rho V_2(l)|\right) \\
&\qquad \le \left(\sum_{l\in\Lambda} \sum_{\rho\in\Lambda\setminus\{0\}} |V_1(l)|^2 F_l(U_\Lambda)^2 e^{-\gamma|\rho|}\right)^{1/2} \\
&\qquad\qquad\qquad \cdot \left(\sum_{l\in\Lambda} \sum_{\rho\in\Lambda\setminus\{0\}} e^{-\gamma|\rho|} |D_\rho V_2(l)|^2\right)^{1/2} \\
&\qquad \le C \|V_1\|_{\ell^\infty(\Lambda)} \|F(U_\Lambda)\|_{\ell^2} \|\nabla V_2\|_\gamma \\
&\qquad \le C \|\nabla U_\Lambda\|_{\ell^2(\Lambda)} \|\nabla V_1\|_{\ell^2(\Lambda)} \|\nabla V_2\|_{\ell^2(\Lambda)}.
\end{aligned}
$$

Renormalisation Sketch (*)

Hence for $V_1, V_2 \in \mathcal{U}^{1,2}$

$$
\begin{aligned}
|\langle \delta^2 \mathcal{E}(U_\Lambda) V_1, V_2 \rangle| &\le |\langle \delta^2 (\mathcal{E}(U_\Lambda) - \mathcal{E}(0)) V_1, V_2 \rangle| + |\langle \delta^2 \mathcal{E}(0) V_1, V_2 \rangle| \\
&\le C(1 + \|\nabla U_\Lambda\|_{\ell^2(\Lambda)}) \|\nabla V_1\|_{\ell^2(\Lambda)} \|\nabla V_2\|_{\ell^2(\Lambda)}.
\end{aligned}
$$

Renormalisation: for $U_\Lambda \in \mathcal{U}^c$

$$
\begin{aligned}
\mathcal{E}(U_\Lambda) &= \mathcal{E}(0) + \langle \delta \mathcal{E}(0), U_\Lambda \rangle + \int_0^1 (1-t) \langle \delta^2 \mathcal{E}(tU_\Lambda) U_\Lambda, U_\Lambda \rangle \, \mathrm{d}t \\
&= \int_0^1 (1-t) \langle \delta^2 \mathcal{E}(tU_\Lambda) U_\Lambda, U_\Lambda \rangle \, \mathrm{d}t.
\end{aligned}
$$

So

$$
|\mathcal{E}(U_\Lambda)| \le C \left(1 + \|\nabla U_\Lambda\|_{\ell^2(\Lambda)}\right) \|\nabla U_\Lambda\|^2_{\ell^2(\Lambda)},
$$

hence $\mathcal{E}$ can be continuously extended to $\mathcal{U}^{1,2}$. Similarly, this can be used to show $\mathcal{E}^d$ can also be extended to $\mathcal{U}^{1,2}$.

Summary

- Exponential estimates.
  - Estimates for compact displacements.
  - Change of variables, global L^2 estimates.
  - Decay of displacement implies decay of correctors.
- Exploiting lattice symmetries for $U_\Lambda = 0$, translational invariance for $U_\Lambda \in \mathcal{U}^{1,2}$, equivalence of norms and embeddings of $\mathcal{U}^{1,2}$.
- Renormalisation implies the minimisation problems (1) are well-defined.

Outlook:

- Approximating the global minimisation problem by a finite problem. Numerical simulations.
- Dislocations.

Thank you for your attention!