

Local Defects in the Thomas-Fermi-von Weiszäcker Theory of Crystals.

Faizan Nazar
working with Christoph Ortner

Many Body Quantum Systems

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Mathematics and Statistics
Centre for Doctoral Training

THE UNIVERSITY OF
WARWICK

Motivation - Defects in Lattices

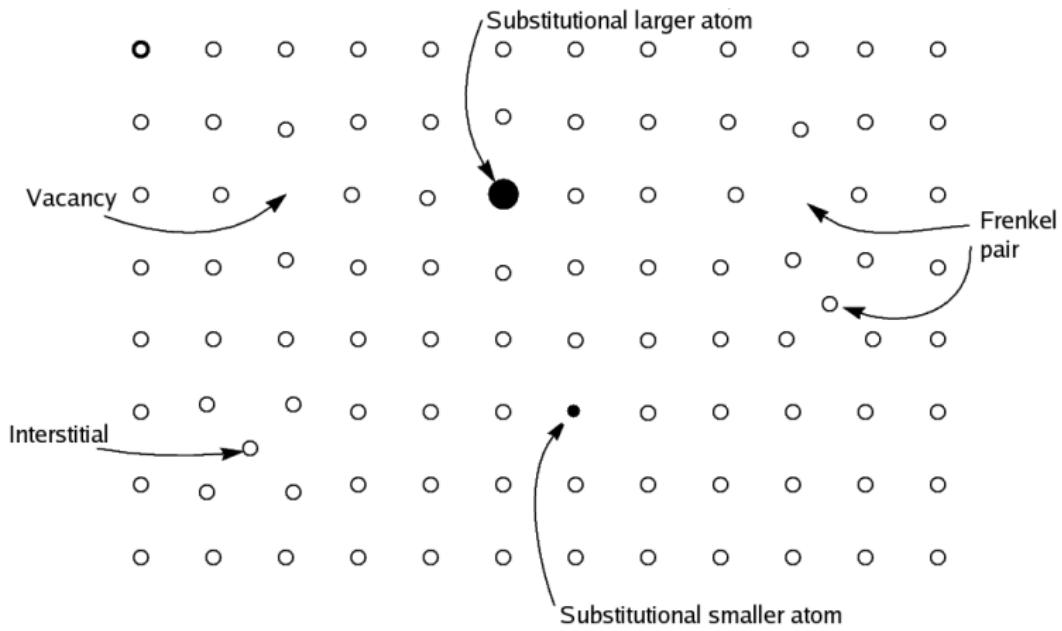


Image by Kai Nordlund

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- ▶ Periodic nuclear density

$$m_0(x) = \sum_{l \in \Lambda} \eta(x - l).$$

- ▶ Defective nuclear density

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1. Nuclear defect - $\rho_{\text{def}}^{\text{nuc}} \in C_c^\infty(B_R(0))$,
2. Nuclear displacement - $U_\Lambda : \Lambda \rightarrow \mathbb{R}^3$, satisfying $U_\Lambda \in \mathcal{W}^{1,2}(\Lambda)$:

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

The TFW Energy

The Thomas-Fermi-von Weiszäcker energy functional is defined as

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

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The minimiser (u, ϕ) is unique and satisfies

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

Existence and uniqueness is shown in [C/LB/L].

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$$(u_1, \phi_1)$$

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We apply a change of variables argument to compare (u_0, ϕ_0) with (u_1, ϕ_1) .

Residual Estimates

First, we interpolate $\text{Id} + U_\Lambda$ from Λ to \mathbb{R}^3 . This gives a bijective deformation field $Y \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$ and $J = \det(\nabla Y)$.

Now define the predictors

$$\tilde{u} = u_0 \circ Y^{-1} J^{-1/2}, \quad \tilde{\phi} = \phi_0 \circ Y^{-1}.$$

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The residual terms $u_1 - \tilde{u}, \phi_1 - \tilde{\phi}$ satisfy

$$\begin{aligned} -\Delta(u_1 - \tilde{u}) + \frac{5}{3}(u_1^{7/3} - \tilde{u}^{7/3}) - \phi_1 u_1 + \tilde{\phi} \tilde{u} &= g_1, \\ -\Delta(\phi_1 - \tilde{\phi}) &= 4\pi(\tilde{u}^2 - u_1^2) + g_2 + 4\pi\rho_{\text{def}}^{\text{nuc}}, \end{aligned}$$

where g_1, g_2 satisfy for each $k \in \mathbb{N}$

$$\|g_1\|_{H^k(\mathbb{R}^3)} + \|g_2\|_{H^k(\mathbb{R}^3)} \leq C_k \|\nabla U_\Lambda\|_{\ell^2(\Lambda)}.$$

Main Estimate

By adapting the proof of uniqueness from [C/LB/L], we obtain

Theorem

For each $k \in \mathbb{N}$, for all $\xi \in C_c^\infty(\mathbb{R}^3)$

$$\begin{aligned} & \sum_{|\alpha| \leq k} \int \left(|\partial^\alpha(u_1 - \tilde{u})|^2 + |\partial^\alpha(\phi_1 - \tilde{\phi})|^2 \right) \xi^2 \\ & \leq C_k \sum_{|\alpha| \leq k} \int \left(|\partial^\alpha g_1|^2 + |\partial^\alpha g_2|^2 + |\partial^\alpha \rho_{\text{def}}^{\text{nuc}}|^2 \right) \xi^2 \\ & \quad + C_k \int \left((u_1 - \tilde{u})^2 + (\phi_1 - \tilde{\phi})^2 \right) |\nabla \xi|^2. \end{aligned}$$

Additional Estimates

- ▶ Sending $\xi \rightarrow 1$ gives

$$\|u_1 - \tilde{u}\|_{H^k(\mathbb{R}^3)} + \|\phi - \tilde{\phi}\|_{H^k(\mathbb{R}^3)} \leq C_k (\|\nabla U_\Lambda\|_{\ell^2(\Lambda)} + \|\rho_{\text{def}}^{\text{nuc}}\|_{H^k(\mathbb{R}^3)}).$$

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- ▶ Suppose that $|\nabla U_\Lambda(I)| \leq C(1 + |I|)^{-d}$, then

$$|(u_1 - \tilde{u})(x)| + |(\phi_1 - \tilde{\phi})(x)| \leq C(1 + \|\rho_{\text{def}}^{\text{nuc}}\|_{L^2(\mathbb{R}^3)})(1 + |x|)^{-d}.$$

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- ▶ Alternatively, suppose $U_\Lambda(I) = 0$ for $|I| > R$, then there exists $\gamma > 0$ such that

$$|(u_1 - \tilde{u})(x)| + |(\phi_1 - \tilde{\phi})(x)| \leq C_R (\|\nabla U_\Lambda\|_{\ell^2(\Lambda)} + \|\rho_{\text{def}}^{\text{nuc}}\|_{L^2(\mathbb{R}^3)}) e^{-\gamma|x|}.$$

Consider the two energy differences

$$\begin{aligned}\mathcal{E}^0(V_\Lambda) &= E^{\text{TFW}}(u_V, m_V) - E^{\text{TFW}}(u_0, m_0), \\ \mathcal{E}^{\text{def}}(V_\Lambda) &= E^{\text{TFW}}(u_V, m_V + \rho_{\text{def}}^{\text{nuc}}) - E^{\text{TFW}}(u_0, m_0).\end{aligned}$$

They are well-defined for any $V_\Lambda \in \mathcal{W}^{1,2}(\Lambda)$

$$\begin{aligned}|\mathcal{E}^0(V_\Lambda)| &\leq C \|\nabla V_\Lambda\|_{\ell^2(\Lambda)}, \\ |\mathcal{E}^{\text{def}}(V_\Lambda)| &\leq C(\|\nabla V_\Lambda\|_{\ell^2(\Lambda)} + \|\rho_{\text{def}}^{\text{nuc}}\|_{L^2(\mathbb{R}^3)}).\end{aligned}$$

Similarly, we can also estimate the forcing and Hessian for both \mathcal{E}^0 , and \mathcal{E}^{def} .

Outlook

We wish to show the existence of a local minimiser U_Λ of \mathcal{E}^{def} and prove decay estimates for U_Λ .

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Thanks for your attention!