Rigorous Kohn–Sham Inversion for Solids

Towards Reliable Exchange-Correlation Potentials

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Acknowledgements

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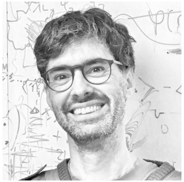

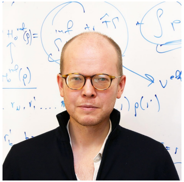

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Outline

The Inverse Kohn–Sham Problem

Interacting electrons

$$-\frac{1}{2}\sum_j \nabla_j^2 + \sum_{k<j} w(\mathbf{r}_j - \mathbf{r}_k) + \sum_j v_{\mathrm{ext}}(\mathbf{r}_j)$$

ρ_{gs}

Non-interacting electrons (KS system)

$$-\frac{1}{2}\sum_j \nabla_j^2 + \sum_j [v_{\mathrm{ext}}(\mathbf{r}_j) + v_{\mathrm{H}}(\mathbf{r}_j) + v_{\mathrm{xc}}(\mathbf{r}_j)]$$

The inverse problem: Given a $\rho_{\mathrm{gs}}(\mathbf{r})$, what is $v_{\mathrm{xc}}(\mathbf{r})$?

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The Periodic Setting

Densities $\rho \in \mathcal{X}_{\mathrm{aff}}$ ⟵ homogeneous periodic Sobolev spaces
Potentials $v \in \mathcal{X}^*$ (Hilbert spaces)

$$\|\rho\|^2_{\mathcal{X}_{\mathrm{aff}}} = \sum_{\mathbf{G}\neq 0} \frac{|\widehat{\rho}_{\mathbf{G}}|^2}{|\mathbf{G}|^2} \qquad \|v\|^2_{\mathcal{X}^*} = \sum_{\mathbf{G}\neq 0} |\mathbf{G}|^2 |\widehat{v}_{\mathbf{G}}|^2$$

The *duality mapping* $J : \mathcal{X}_{\mathrm{aff}} \to \mathcal{X}^*$,

$$J[\rho](\mathbf{r}) = \sum_{\mathbf{G}\neq 0} \frac{1}{|\mathbf{G}|^2} \widehat{\rho}_{\mathbf{G}} e_{\mathbf{G}}(\mathbf{r})$$

$$E_{\mathrm{H}}(\rho) = \frac{1}{2} \|\rho\|^2_{\mathcal{X}_{\mathrm{aff}}}$$

Bakkestuen et al. *In preparation* (2026)

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Moreau–Yosida Regularisation

Let $\mathcal{F} : \mathcal{X}_{\mathrm{aff}} \to \mathbb{R} \cup \{+\infty\}$ be proper, convex, and lower semicontinous.
For $\varepsilon > 0$, the *Moreau–Yosida regularisation* is

$$\mathcal{F}^{\varepsilon}(\rho) = \inf_{\sigma \in \mathcal{X}_{\mathrm{aff}}} \left\{ \mathcal{F}(\sigma) + \frac{1}{2\varepsilon} \|\sigma - \rho\|_{\mathcal{X}}^2 \right\}$$

Unique optimiser: *the proximal point*

$$\operatorname*{prox}_{\varepsilon\mathcal{F}}(\rho) = \operatorname*{argmin}_{\sigma \in \mathcal{X}_{\mathrm{aff}}} \left\{ \mathcal{F}(\sigma) + \frac{1}{2\varepsilon} \|\sigma - \rho\|_{\mathcal{X}}^2 \right\}$$

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The Inversion Scheme

The Guiding Functional

Goal: Given ρ_{gs}, determine v_{xc}

$$\mathcal{F}(\rho) = T(\rho) + E_{\mathrm{H}}(\rho) + \int_\Omega v_{\mathrm{ext}}(\mathbf{r})\rho(\mathbf{r})\,\mathrm{d}\mathbf{r}$$

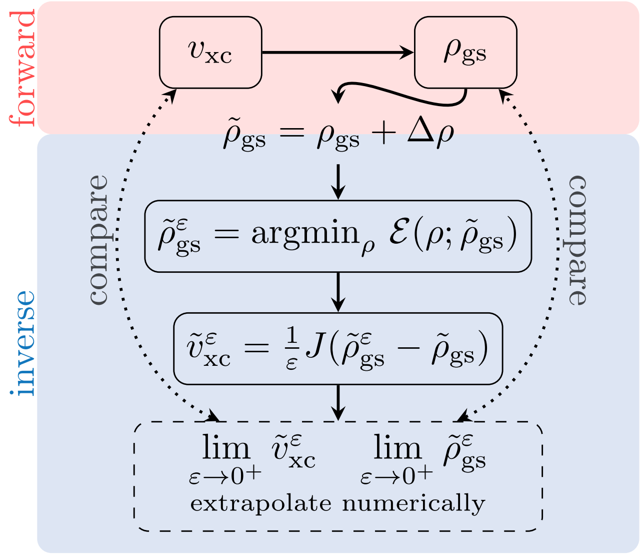
Minimise $\quad \mathcal{E}(\rho;\rho_{\mathrm{gs}}) = \mathcal{F}(\rho) + \frac{1}{2\varepsilon}\|\rho - \rho_{\mathrm{gs}}\|_{\mathcal{X}}^2$

$$\rho^\varepsilon(\mathbf{r}) = \operatorname*{prox}_{\varepsilon\mathcal{F}}(\rho_{\mathrm{gs}})(\mathbf{r}) \qquad v_{\mathrm{xc}}^\varepsilon(\mathbf{r}) = \frac{1}{\varepsilon}J(\rho^\varepsilon - \rho_{\mathrm{gs}})(\mathbf{r})$$

$$v_{\mathrm{xc}}(\mathbf{r}) = \lim_{\varepsilon\to0^+} v_{\mathrm{xc}}^\varepsilon(\mathbf{r}) = \lim_{\varepsilon\to0^+}\frac{1}{\varepsilon}J(\rho^\varepsilon - \rho_{\mathrm{gs}})(\mathbf{r})$$

Penz et al. *Electron. Struct.* **5**, 014009 (2023)
Herbst et al. *Phys. Rev. B* **111**, 205143 (2025)

The Inversion Algorithm



Planewave KS-DFT:

$$\Phi = (\varphi_1, \dots, \varphi_N)$$

Minimise $\mathcal{E}(\Phi;\ \rho_{\rm gs})$

$$\rho_\Phi(\mathbf{r}) = \sum_{i=1}^{N} |\varphi_j(\mathbf{r})|^2$$

DFTK

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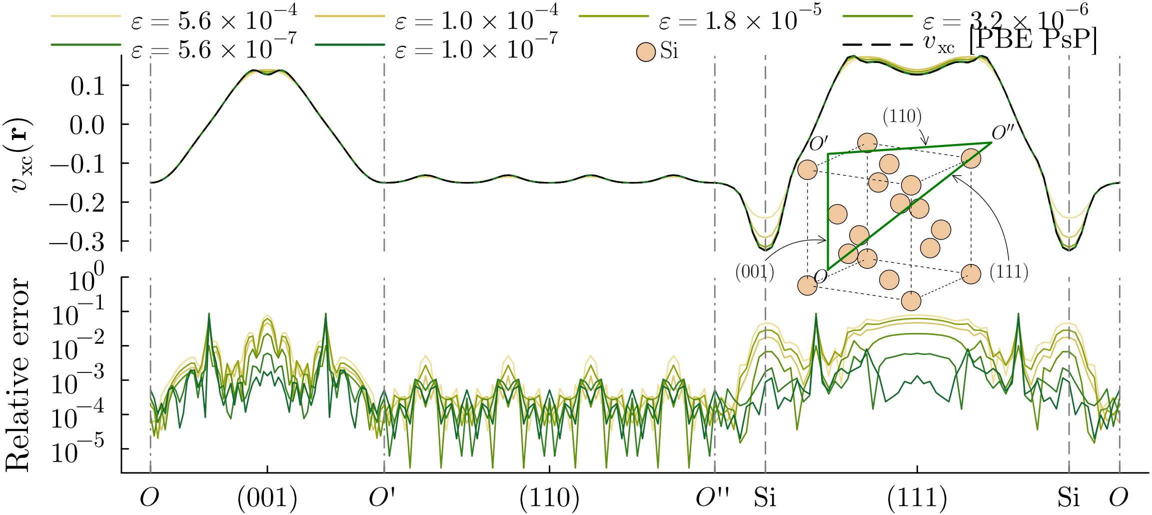
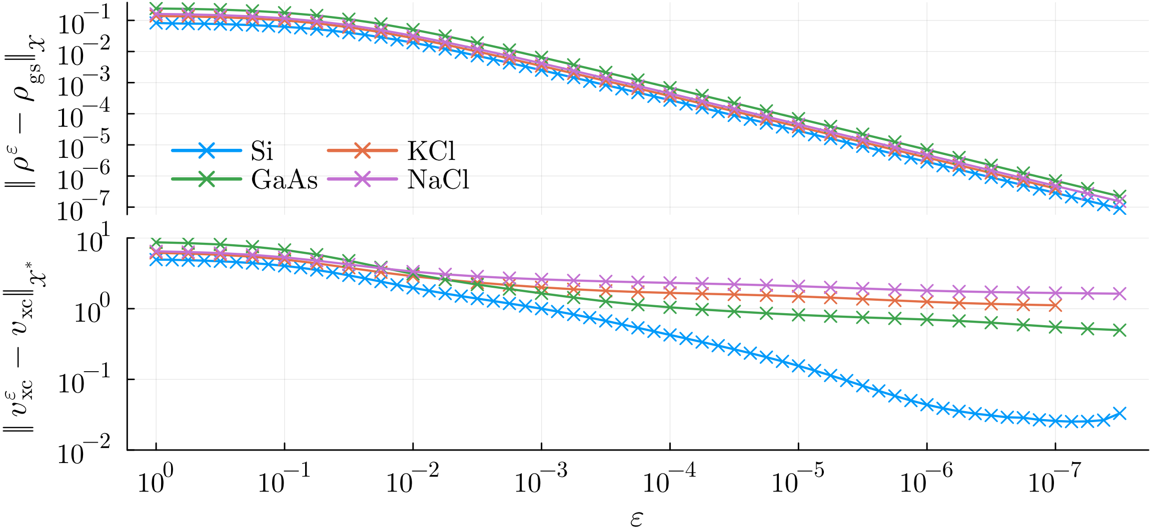
Bulk Silicon



Implementation: github.com/mfherbst/supporting-my-inversion

Convergence



Error Bounds

The proximal mapping is non-expansive,

$$\left\| \operatorname*{prox}_{\varepsilon\mathcal{F}}(\rho) - \operatorname*{prox}_{\varepsilon\mathcal{F}}(\widetilde{\rho}) \right\|_{\mathcal{X}} \leq \|\rho - \widetilde{\rho}\|_{\mathcal{X}}, \quad \forall \rho, \widetilde{\rho} \in \mathcal{X}_{\mathrm{aff}}$$

Consider inexact references:

$$\widetilde{\rho}_{\mathrm{gs}} = \rho_{\mathrm{gs}} + \Delta\rho$$

The *total error*

$$\begin{aligned} \|v_{\mathrm{xc}} - \widetilde{v}^{\varepsilon}_{\mathrm{xc}}\|_{\mathcal{X}^*} &\leq \|v_{\mathrm{xc}} - v^{\varepsilon}_{\mathrm{xc}}\|_{\mathcal{X}^*} + \|v^{\varepsilon}_{\mathrm{xc}} - \widetilde{v}^{\varepsilon}_{\mathrm{xc}}\|_{\mathcal{X}^*} \\ &\leq \|v_{\mathrm{xc}} - v^{\varepsilon}_{\mathrm{xc}}\|_{\mathcal{X}^*} + \frac{1}{\varepsilon}\|\Delta\rho\|_{\mathcal{X}} \end{aligned}$$

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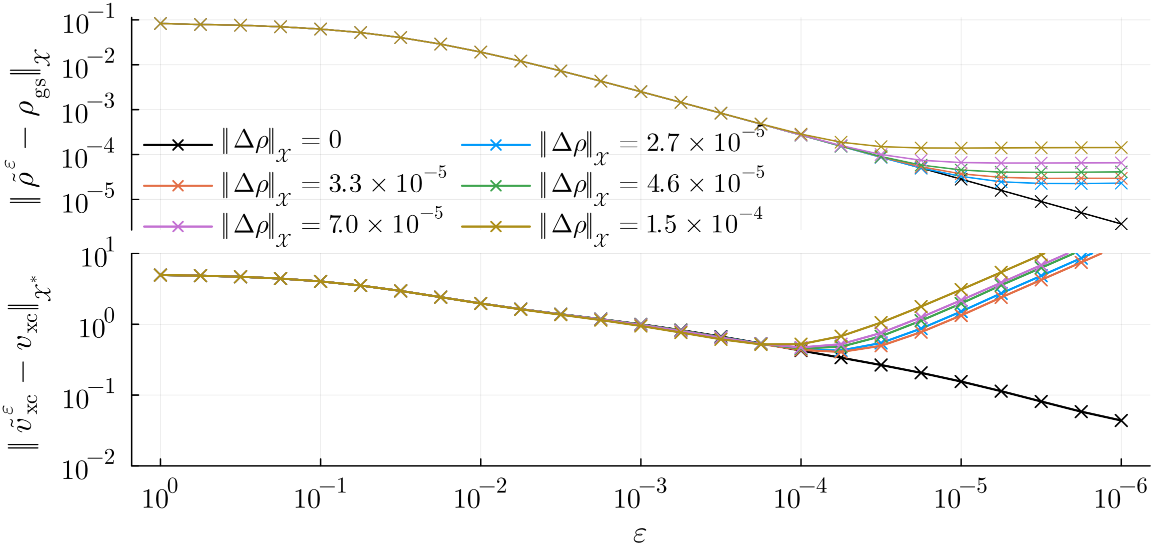
Bulk Silicon



Conclusions

- Mathematically rigorous inversion scheme
- Offers error estimates
- Practical use case of Moreau–Yosida regularisation

Outlook

- More complicated systems
- Molecular systems
- Reference densities from other sources
- Further error analysis

References

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3. **Herbst, M. F.** *mfherbst/supporting-my-inversion: v0.1.0.* 2025. https://zenodo.org/doi/10.5281/zenodo.14894065.
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Thank you for your attention!

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