A Moreau–Yosida-Based Kohn–Sham Inversion Scheme

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Acknowledgements

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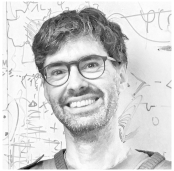

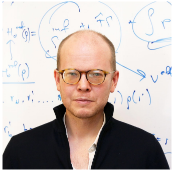

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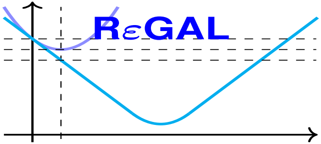
Funded under ERC StG No. 101041487 REGAL



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Established by the European Commission

Main References

To appear on arXiv (soon)

PHYSICAL REVIEW B **111**, 205143 (2025)

Kohn-Sham inversion with mathematical guarantees

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(Received 7 September 2024; revised 3 March 2025; accepted 6 May 2025; published 28 May 2025)

We use an exact Moreau-Yosida regularized formulation to obtain the exchange-correlation potential for periodic systems. We reveal a profound connection between rigorous mathematical principles and efficient numerical implementation, which marks a successful application of a Moreau-Yosida-based inversion for physical systems. We develop a mathematically rigorous inversion algorithm that is demonstrated for representative bulk materials, specifically bulk silicon, gallium arsenide, and potassium chloride. Our inversion algorithm allows the construction of rigorous error bounds that we are able to verify numerically. This unlocks a pathway to analyze Kohn-Sham inversion methods, which we expect in turn to foster mathematical approaches for developing approximate functionals.

DOI: 10.1103/PhysRevB.111.205143

I. INTRODUCTION

Density-functional theory (DFT) simulations are an indispensable tool in chemistry, materials science, and solid-state physics [1–3]. In this theory, the unknown is the electronic density $\rho(\mathbf{r})$ instead of the full many-body wavefunction, making computations substantially more tractable [4]. However, one of the key ingredients of DFT, the universal density functional, is not known explicitly [5]. One therefore usually employs the Kohn-Sham (KS) formulation [6], where all unknowns of DFT are collected into the exchange-correlation (xc) functional, which is subsequently approximated. Substantial work has been devoted to developing accurate xc functional approximations [7]. Although DFT is in principle exact, and despite significant advancements, KS-DFT still faces challenges in certain physical contexts. Notable difficulties include accurately describing processes involving fractional electronic charge, such as dissociation or charge-transfer excitations [8–10], as well as addressing the well-known band gap problem, where semiconductor band gaps are underestimated [11–15]. Developing better xc functional approximations thus remains a major research thrust [16]. One obstacle is a lack in mathematical understanding between the exact universal density functional and common approximations [3], making the rigorous construction of new and better functionals hard.

In this paper, we focus on KS inversion [17–43], which has been suggested as a tool to aid the construction of xc functionals [36,40,42]. In 1994, van Leeuwen and Baerends [24] utilized an inversion scheme to improve approximations to the KS potential. More recently, there has been considerable interest in KS inversion, leading for example to targeted software packages such as *n2v* [44] and *KS-pies* [45]. Both implement a variety of established inversion schemes, beyond the van-Leeuwen-Baerends method including the Zhao-Morrison-Parr [22] (ZMP) and Wu-Yang [26] methods. While initial exploration of KS inversion has focused on isolated systems and molecules, recent studies have begun to tackle a wide range of solid-state systems as well [43,46]. In contrast to the standard KS formulation, where one is equipped with an approximate xc potential and determines the density from a variational principle (forward problem), KS inversion does the reverse: Given a ground-state density one seeks the exact xc potential v_{xc}, which reproduces the density in an auxiliary noninteracting setting. Unfortunately, KS inversion is far less studied than the forward KS-DFT problem. Additionally, the development of a robust and efficient numerical scheme for KS inversion remains an open challenge [40,42,44,45,47,48].

In a recently established result [49], the xc potential has been obtained as a mathematical limit within the Moreau-Yosida (MY) regularized formulation of DFT [50–54]. This limit involves first finding the *proximal density* (of a ground-state density) and then utilizing the duality map between the density and potential spaces. This previously unexplored link is extremely promising as MY regularization deals with the

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2469-9950/2025/111(20)/205143(10) 205143-1 Published by the American Physical Society

Moreau–Yosida-based Kohn–Sham Inversion for Periodic Systems

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(Dated: 15 May 2026)

Density-potential inversion for periodic systems within Moreau–Yosida-regularised density-functional theory is investigated, both theoretically and numerically. We develop the framework in a periodic homogeneous Sobolev space and use it to recover the exchange-correlation potential of Kohn–Sham theory through a limiting procedure. A key analytical ingredient is the proof of lower semicontinuity of the non-interacting kinetic-energy functional in the chosen topology. The proximal mapping, together with its algorithmic evaluation, plays a central role in the resulting inversion scheme. Numerical experiments illustrate the performance and properties of the method for both the Kohn–Sham and Gross–Pitaevskii equations.

I. INTRODUCTION

Density-functional theory (DFT) calculations are an indispensable tool in theoretical and practical applications of the many-body electronic Schrödinger equation across disciplines such as chemistry, materials science, and solid-state physics [1–3]. Its central variable is the one-particle density, here denoted $\rho(\mathbf{r})$, $\mathbf{r} \in \Omega \subseteq \mathbb{R}^d$, where for the standard formulation of DFT $\Omega = \mathbb{R}^3$. Practical DFT calculations are performed almost exclusively within the Kohn–Sham (KS) framework, in which the sought-after ground-state density $\rho_{gs}(\mathbf{r})$ of an interacting system is assumed to be a solution to a non-interacting problem as well. This fictitious KS system is determined by the effective KS potential v_{KS}, a local potential responsible for generating the *same* ground-state density of the original, interacting system.

The universal density functional $F(\rho)$ encapsulates all many-body effects such that the ground-state energy for a given external scalar potential $v : \Omega \to \mathbb{R}$ can be written as

$$E(v) = F(\rho_{gs}) + \langle v, \rho_{gs} \rangle, \qquad \langle v, \rho \rangle = \int_\Omega v(\mathbf{r})\rho(\mathbf{r})\mathrm{d}\mathbf{r}.$$

The explicit form of F is unknown in general. Applications of Kohn–Sham density-functional theory (KS-DFT) rely on approximations to the functional from which the effective KS potential is derived. Over the years, substantial efforts have been devoted to obtaining accurate approximations [4] which typically address the *exchange-correlation* (xc) energy E_{xc} in the decomposition

$$F(\rho) = T(\rho) + E_H(\rho) + E_{xc}(\rho). \tag{1}$$

Here $T(\rho)$ is the non-interacting kinetic-energy functional and $E_H(\rho)$ is the (direct) Hartree energy. Given the potential of the physical system v, the KS potential is typically split into $v_{KS} = v + v_H + v_{xc}$, where v_H is the Hartree (electrostatic) potential and v_{xc} is the xc potential that must be approximated. Although DFT in general and KS-DFT in particular are exact reformulations of the many-body Schrödinger equation and significant advancements have been made over the years, KS-DFT with the current functional approximations remains unable to predict certain physical processes. Inaccurate approximations to v_{xc} are important sources of errors in KS-DFT calculations, e.g., band-gap underestimation [5–9] and self-interaction errors [10]. Developing improved functional approximations continues to be a central research focus [11]. A key difficulty lies in the limited mathematical insight into the relationship between the exact universal density functional and the widely used approximations [3], which hampers the systematic design of approximate functionals.

To obtain an effective KS potential corresponding to a given interacting ground-state density is a highly non-trivial task [12; 13]. We aim to shed more light on this issue by both mathematically and numerically addressing this inverse KS problem: given knowledge of the exact (or near-exact) ground-state density, reconstruct the effective KS

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Outline

Density-Functional Theory

$$\widehat{H} = \underbrace{-\frac{1}{2}\sum_j \nabla_j^2 + \frac{1}{2}\sum_{k\neq j}\frac{1}{|\mathbf{r}_j - \mathbf{r}_k|}}_{\widehat{H}_0} + \sum_j v(\mathbf{r}_j)$$

$$\begin{aligned} E(v) &= \inf_{\psi} \langle\psi|\widehat{H}|\psi\rangle \\ &= \inf_{\rho} \{F(\rho) + \langle v,\, \rho\rangle\} \end{aligned}$$

$$\begin{aligned} F(\rho) &= \sup_{v} \{E(v) - \langle v,\, \rho\rangle\} \\ &= \inf_{\Gamma\mapsto\rho} \operatorname{Tr} \widehat{H}_0\Gamma \end{aligned}$$

$$\langle v,\, \rho\rangle = \int v(\mathbf{r})\rho(\mathbf{r})\,\mathrm{d}\mathbf{r}$$

The Inverse Kohn–Sham Problem

Interacting electrons

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

ρ_{gs}

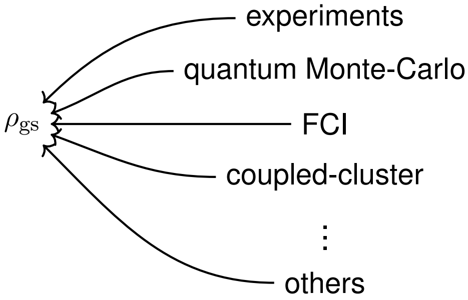
Non-interacting electrons (KS system)

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

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

The Inverse Kohn–Sham Problem

Given a ρ_{gs}, determine v_{xc}



Better understanding of $F(\rho)$

Novel approximations to $F(\rho)$

Previous Inversion Schemes

1994: van Leeuwen and Baerends

$$v_{\mathrm{xc}}(\mathbf{r}) = \rho^{1/3}(\mathbf{r}) f\left[|\nabla\rho|/\rho^{4/3}\right](\mathbf{r})$$

1994: Zhao, Morrison, and Parr (ZMP)

$$v_{\mathrm{xc}} = \lim_{\lambda\to+\infty} \lambda \int \frac{\rho(\mathbf{r}') - \rho_0(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}\mathbf{r}'$$

2003: Wu and Yang

$$v_{\mathrm{KS}}(\mathbf{r}) = v_{\mathrm{ext}}(\mathbf{r}) + v_0(\mathbf{r}) + \sum_t b_t g_t(\mathbf{r})$$

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van Leeuwen and Baerends *Phys. Rev. A* **49**, 2421 (1994)
Zhao, Morrison, and Parr *Phys. Rev. A* **50**, 2138 (1994)
Wu and Yang *J. Chem. Phys.* **118**, 2498–2509 (2003)

Moreau–Yosida Regularisation

Assumption

A density space X is a strictly convex and reflexive real Banach space that contains $\mathcal{I}_N$, and the dual space X^*, the space of potentials, is strictly convex. The functional F is proper, convex, and lower semicontinuous (l.s.c.) with respect to the topology of X.

Definition

Let X be uniformly convex and $F : X \to \mathbb{R} \cup \{+\infty\}$ convex and l.s.c. functional. For some $\varepsilon > 0$, the *Moreau–Yosida regularisation* of F is

$$F^{\varepsilon}(\rho) = \inf_{\sigma \in X} \left\{ F(\sigma) + \frac{1}{2\varepsilon} \|\sigma - \rho\|_X^2 \right\}.$$

The Proximal Point

Lemma

If X and F satisfy Assumption, then for every $\rho \in X$ and $\varepsilon > 0$ there exists a unique minimiser $\rho^\star \in X$ of $F(\sigma) + \frac{1}{2\varepsilon}\|\sigma - \rho\|_X^2$.

Definition

The *proximal mapping* $\Pi_f^\varepsilon : X \to X$ is defined as

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

and $\Pi_F^\varepsilon(\rho)$ is referred to as the proximal point or proximal density.

A Lossless Regularisation

$$E^{\varepsilon}(v) = \inf_{\rho \in X} \{F^{\varepsilon}(\rho) + \langle v, \rho \rangle\}$$

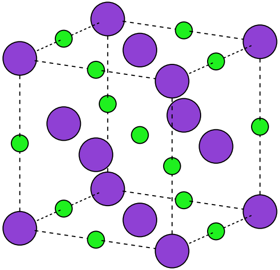
$$E^{\varepsilon}(v) = E(v) - \frac{\varepsilon}{2}\|v\|_{X^*}^2$$

Consequence of infimal convolution

$$E(\text{concave}) \leftrightarrow F(\text{convex})$$

Inversion Scheme

Periodic Systems



$$X = H^{-1}_{\mathrm{per}}(\Omega, \mathbb{C}) \qquad X^* = H^{1}_{\mathrm{per}}(\Omega, \mathbb{C})$$

Periodic Sobolev spaces

$$\|u\|^2_{H^s_{\mathrm{per}}} = \sum_{\mathbf{G}} (1 + |\mathbf{G}|^2)^s |\widehat{u}_{\mathbf{G}}|^2$$

The *duality mapping* $J : X \to X^*$,

$$J[\rho](\mathbf{r}) = \sum_{\mathbf{G}} \frac{\widehat{\rho}_{\mathbf{G}} e_{\mathbf{G}}(\mathbf{r})}{1 + |\mathbf{G}|^2} = (\mathbf{\Phi} * \rho)(\mathbf{r}) = \int_{\mathbb{R}^3} \frac{\rho(\mathbf{x})}{4\pi|\mathbf{r} - \mathbf{x}|} e^{-|\mathbf{r}-\mathbf{x}|} \, \mathrm{d}\mathbf{x}$$

Cancès, Chakir, and Maday *ESAIM: M2AN* **46**, 341-388 (2012)
Herbst, Bakkestuen, Laestadius *Phys. Rev. B* **111**, 205143 (2025)

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The Periodic Setting I

The Poisson equation

$$\nabla^2 v(\mathbf{r}) = \rho(\mathbf{r}) - \frac{N}{|\boldsymbol{\Omega}|}, \qquad \forall \mathbf{r} \in \boldsymbol{\Omega}$$

$$v(\mathbf{r}) = \sum_{\mathbf{G}\neq 0} \frac{1}{|\mathbf{G}|^2} \widehat{\rho}_{\mathbf{G}} e_{\mathbf{G}}(\mathbf{r}) \quad \rightsquigarrow \quad H^1_{\text{per,hom}}(\boldsymbol{\Omega}) = H^1_{\text{per}}(\boldsymbol{\Omega})/\mathbb{R}$$

The space of potentials:

$$\mathcal{X}^* = \{v : v \in [v] \in H^1_{\text{per,hom}}(\boldsymbol{\Omega}),\ \widehat{v}_{\mathbf{G}=0} = 0\} \qquad \|v\|_{\mathcal{X}^*} = \sqrt{\sum_{\mathbf{G}\neq 0} |\mathbf{G}|^2 |\widehat{v}_{\mathbf{G}}|^2}$$

The space of densities:

$$\mathcal{X}_{\text{aff}} := \left\{ f + \frac{N}{|\boldsymbol{\Omega}|} : f \in H^{-1}_{\text{per,hom}}(\boldsymbol{\Omega}) \right\} \qquad \|\rho\|_{\mathcal{X}_{\text{aff}}} = \left\| \rho - \frac{N}{|\boldsymbol{\Omega}|} \right\|_{\mathcal{X}} = \sqrt{\sum_{\mathbf{G}\neq 0} \frac{|\widehat{\rho}_{\mathbf{G}}|^2}{|\mathbf{G}|^2}}$$

Bakkestuen *et al.* In preparation (2026)

The Periodic Setting II

$$\|\rho\|^2_{\mathcal{X}_{\text{aff}}} = \sum_{\mathbf{G}\neq 0} \frac{|\widehat{\rho}_{\mathbf{G}}|^2}{|\mathbf{G}|^2} \qquad \|v\|^2_{\mathcal{X}^*} = \sum_{\mathbf{G}\neq 0} |\mathbf{G}|^2 |\widehat{v}_{\mathbf{G}}|^2 = \|\nabla v\|^2_{L^2(\Omega)}$$

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

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

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

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Model Functional

Recall

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

Fix $\rho_{\mathrm{gs}} \in \mathcal{X}_{\mathrm{aff}}$ and

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

Minimise

$$\mathcal{E}(\rho\,;\rho_{\mathrm{gs}}) = \mathcal{F}(\rho) + \tfrac{1}{2\varepsilon}\|\rho - \rho_{\mathrm{gs}}\|_{\mathcal{X}}^2 \quad \text{over} \quad \rho \in \mathcal{X}_{\mathrm{aff}} \tag{1}$$

Unique minimiser, the *proximal density:*

$$\rho^\varepsilon = \operatorname*{argmin}_{\rho\in\mathcal{X}_{\mathrm{aff}}} \mathcal{E}(\rho, \rho_{\mathrm{gs}})$$

Barbu and Precubanu, *Convexity and Optimization in Banach Spaces* (2012)

The Exchange-Correlation Potential

Since $\mathcal{F}^\varepsilon(\rho)$ is differentiable,

$$v_{\mathrm{xc}}^\varepsilon = -\frac{\delta \mathcal{F}^\varepsilon}{\delta \rho}[\rho^\varepsilon] = \frac{1}{\varepsilon} J[\rho^\varepsilon - \rho_{\mathrm{gs}}]$$

Exchange-correlation potential

$$v_{\mathrm{xc}}(\mathbf{r}) = \lim_{\varepsilon \to 0^+} v_{\mathrm{xc}}^\varepsilon = \lim_{\varepsilon \to 0^+} \frac{1}{\varepsilon} J[\rho^\varepsilon - \rho_{\mathrm{gs}}]\,(\mathbf{r})$$

Set $\varepsilon = 1/\lambda$

$$v_{\mathrm{xc}}(\mathbf{r}) = \lim_{\lambda \to \infty} \lambda J[\rho^{1/\lambda} - \rho_{\mathrm{gs}}](\mathbf{r}) = \int_{\mathbb{R}^3} \frac{\rho^{1/\lambda}(\mathbf{x}) - \rho_{\mathrm{gs}}(\mathbf{x})}{4\pi|\mathbf{r} - \mathbf{x}|}\,\mathrm{d}\mathbf{x}$$

Penz et al. *Electron. Struct.* **5**, 014009 (2023)
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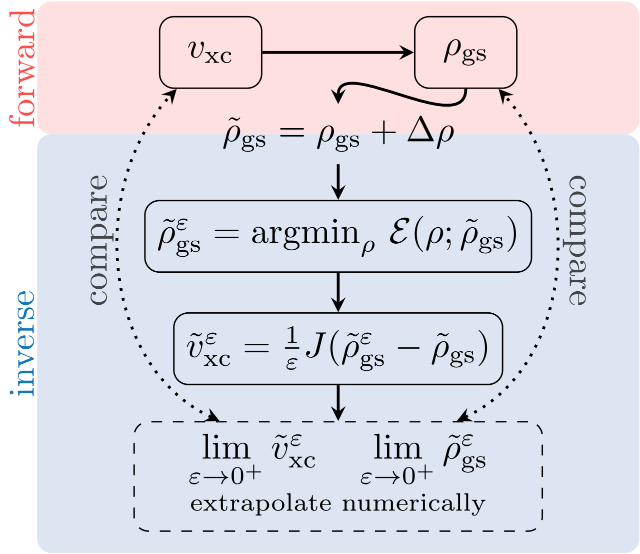
The Inversion Algorithm



Planewave KS-DFT:

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

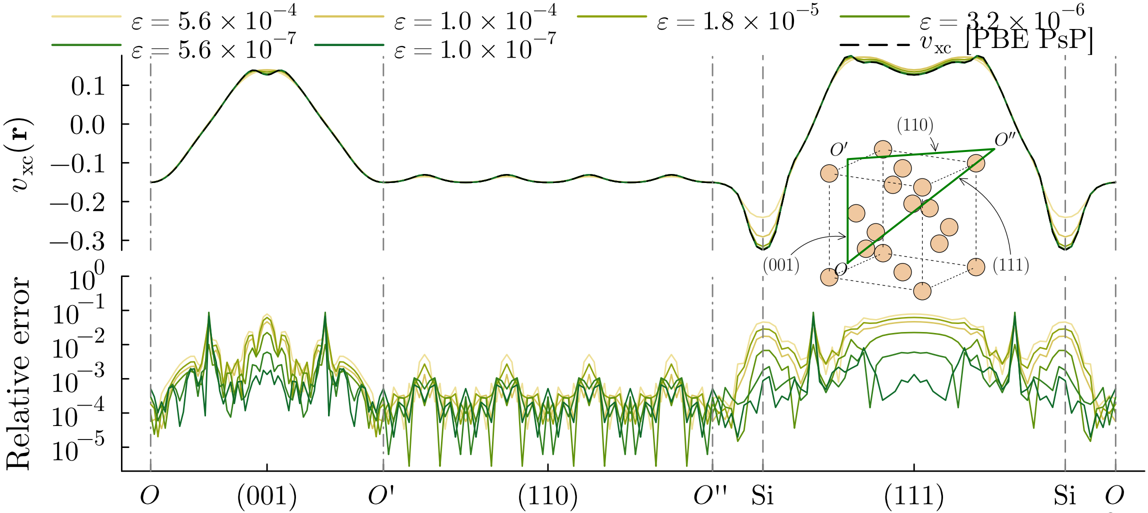
Minimise $\mathcal{E}(\Phi;\ \rho_{\text{gs}})$

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

DFTK

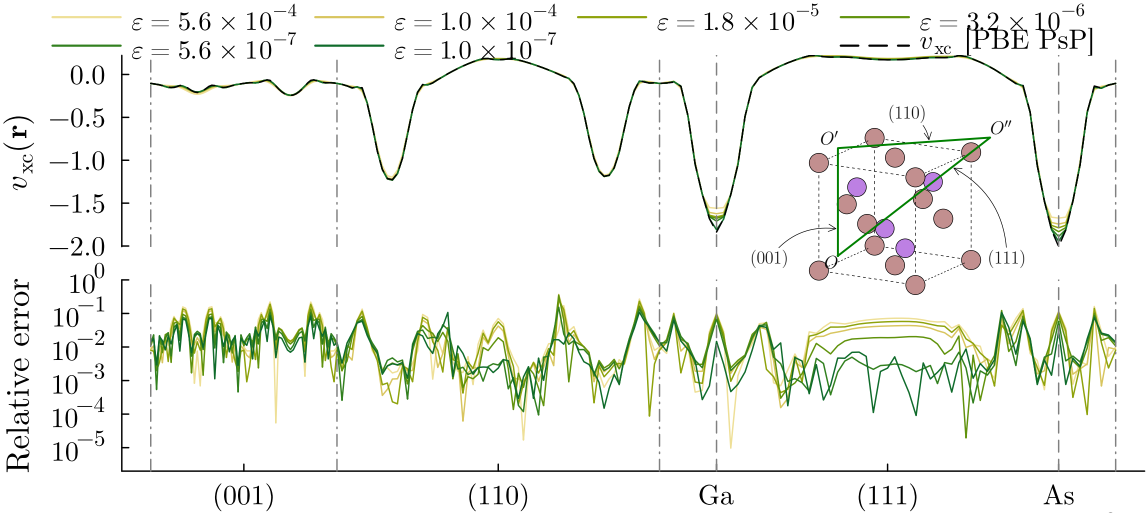
Results

Bulk Silicon

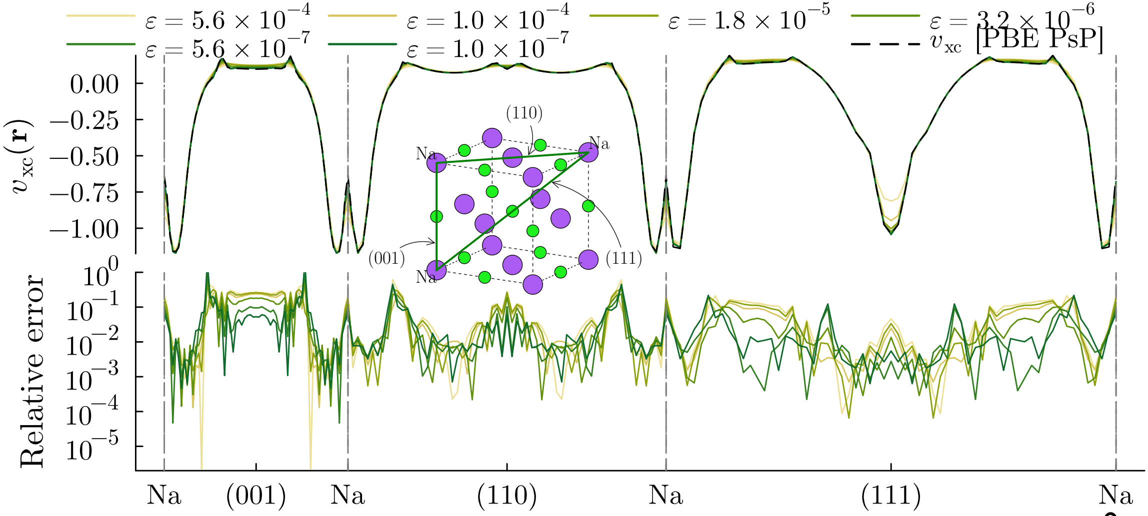


github.com/vebjorhb/MY-periodic-inversion

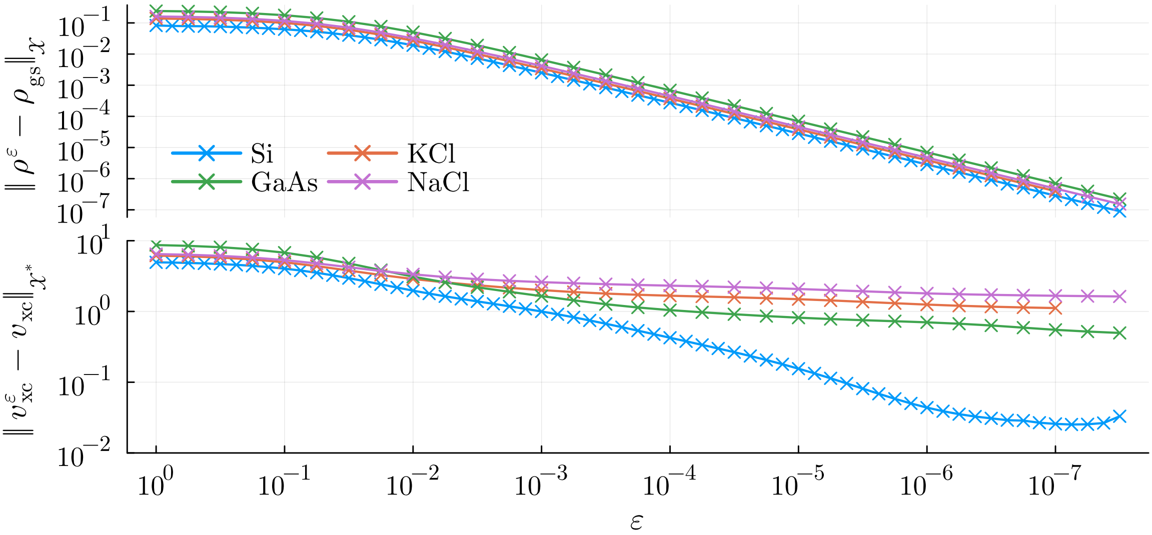
Gallium Arsenide



Sodium Chloride



Convergence



Choice of Guiding Functional

For $\alpha \geq 0$, $\beta, \gamma \in \mathbb{R}$:

$$\mathcal{F}_{\alpha,\beta,\gamma}(\rho) = T(\rho) + \alpha E_{\mathrm{H}}(\rho) + \beta\langle v[\rho_{\mathrm{gs}}],\, \rho\rangle + \gamma\langle v_{\mathrm{ext}},\, \rho\rangle$$

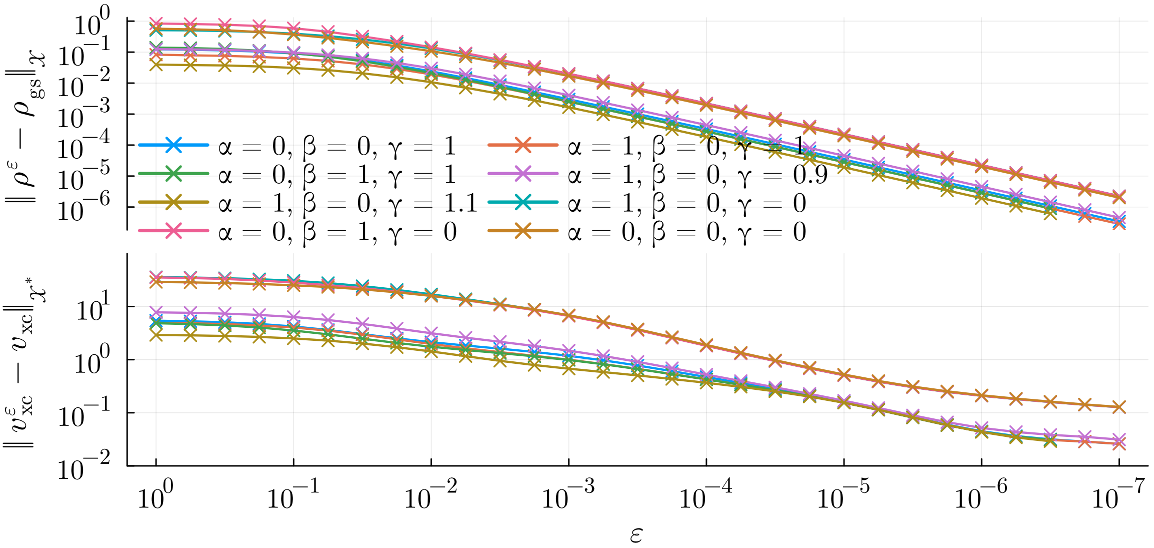
Set $\mu = \frac{\varepsilon}{1+\varepsilon(\alpha-\alpha')} > 0$, then

$$\Pi^{\varepsilon}_{\mathcal{F}_{\alpha,\beta,\gamma}}(\rho) = \Pi^{\mu}_{\mathcal{F}_{\alpha',\beta',\gamma'}}\left(\frac{\mu}{\varepsilon}\rho - \mu(\beta-\beta')\rho_{\mathrm{gs}} - \mu(\gamma-\gamma')J^{-1}(v_{\mathrm{ext}})\right)$$

The term $\frac{1}{\varepsilon}J(\rho^{\varepsilon} - \rho_{\mathrm{gs}})$ targets as $\varepsilon \to 0^{+}$

- the full KS potential if $(\alpha, \beta, \gamma) = (0, 0, 0)$,
- the Hartree-exchange-correlation potential if $(\alpha, \beta, \gamma) = (0, 0, 1)$, and
- the exchange-correlation potential if $(\alpha, \beta, \gamma) = (1, 0, 1)$ or $(0, 1, 1)$.

Choice of Guiding Functional



Error Bounds

The proximal mapping is non-expansive,

$$\|\Pi_F^\varepsilon(\rho) - \Pi_F^\varepsilon(\sigma)\|_{\mathcal{H}} \leq \|\rho - \sigma\|_{\mathcal{H}}, \quad \forall \rho, \sigma \in \mathcal{H}$$

Inexact density:

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

exp. noise

change of basis

truncations

poor convergence

etc.

The *total error*

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

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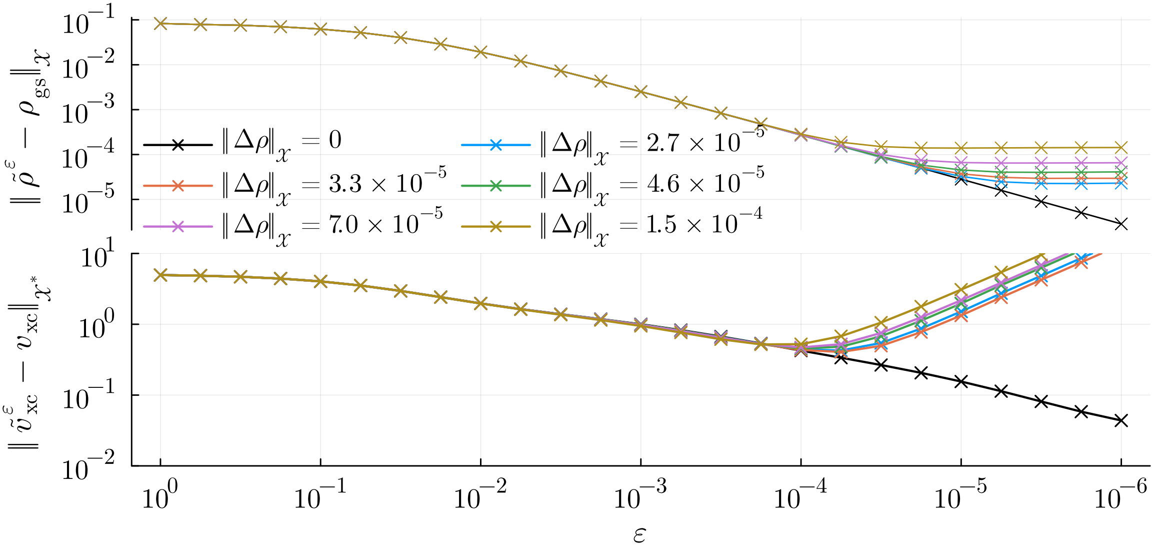
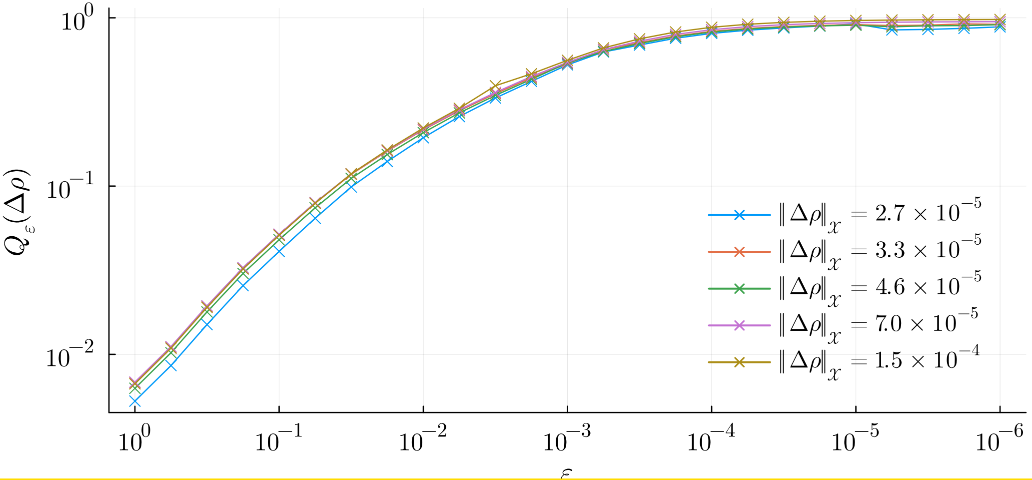
Bulk Silicon



Non-Expansiveness of $\Pi_F^{\varepsilon}(\rho)$

$$\|\rho_{\text{gs}}^{\varepsilon} - \widetilde{\rho}_{\text{gs}}^{\varepsilon}\|_{\mathcal{X}} \leq \|\rho_{\text{gs}} - \widetilde{\rho}_{\text{gs}}\|_{\mathcal{X}} = \|\Delta\rho\|_{\mathcal{X}} \qquad Q_{\varepsilon}(\Delta\rho) = \frac{\|\rho_{\text{gs}}^{\varepsilon} - \widetilde{\rho}_{\text{gs}}^{\varepsilon}\|_{\mathcal{X}}}{\|\Delta\rho\|_{\mathcal{X}}}$$



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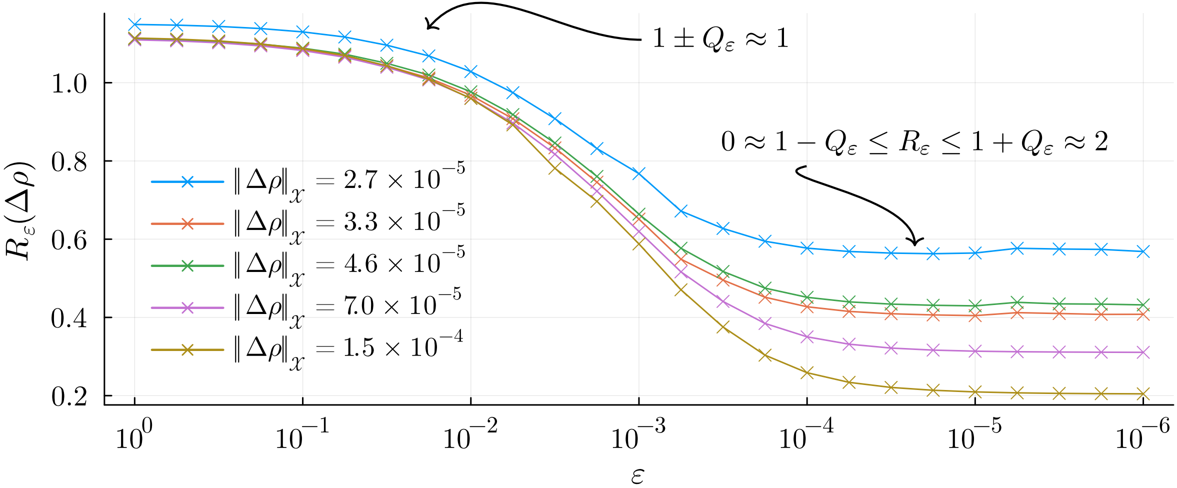
Error Bounds: Inexact Densities

$$\|\widetilde{v}^{\varepsilon}_{\mathrm{xc}} - v^{\varepsilon}_{\mathrm{xc}}\|_{\mathcal{X}^*} \leq \frac{1 + Q_\varepsilon(\Delta\rho)}{\varepsilon}\|\Delta\rho\|_{\mathcal{X}} \qquad R_\varepsilon(\Delta\rho) = \varepsilon\frac{\|\widetilde{v}^{\varepsilon}_{\mathrm{xc}} - v^{\varepsilon}_{\mathrm{xc}}\|_{\mathcal{X}^*}}{\|\Delta\rho\|_{\mathcal{X}}}$$



Conclusions

- Mathematically rigorous inversion scheme
- Rigorous error estimates
- Practical use case of Moreau–Yosida regularisation
- First systems studied: Si, GaAs, KCl, NaCl
- Implemented using `DFTK.jl`

Outlook

- More complicated systems
- Reference densities from other sources
- Further error analysis
- Investigate proximal point algorithms

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Thank you for your attention!

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Choice of Guiding Functional