Regularised Density-Potential Inversion for Periodic Systems

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Acknowledgements

In collaboration with Oliver M. Bohle[1,2], Maryam Lotfigolian[1], André Laestadius[1,2] & Erik I. Tellgren[2].

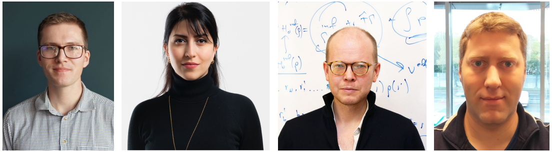

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Table of Contents

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Motivation

- Success of DFT depends on exchange-correlation approximations
- Inverse Kohn–Sham: given ground-state density, find effective potential
- Periodic systems

Theory

Periodic DFT Framework

- Periodic function spaces over the unit cell $\mathcal{C}$

$$\rho \in X = H^{-1}(\mathcal{C}), \quad v \in X^* = H^1(\mathcal{C}) \tag{1}$$

- Born–von Kármán boundary conditions
- Hamiltonian

$$H_\lambda(v) = -\frac{1}{2}\sum_{i=1}^{n} \nabla_i^2 + \sum_{i=1}^{n} v_{\text{ext}}(\vec{r}_i) + \lambda \sum_{i=1}^{n}\sum_{j=1}^{M} w(\vec{r}_i - \vec{r}_j) = T + V + \lambda W \tag{2}$$

- Yukawa interaction w
- Explicit form of the duality map $J : X \to X^*$

$$J(\widehat{\rho})(\mathbf{G}) = \frac{\widehat{\rho}(\mathbf{G})}{\gamma^2 + G^2}, \quad \mathbf{G} \in \mathcal{RL} \tag{3}$$

Moreau–Yosida Regularisation

- Constrained-search universal functional

$$\begin{aligned} F_\lambda(\rho) &= \inf_{\Gamma\mapsto\rho} \operatorname{Tr}\Gamma H_\lambda(0) \\ E_\lambda(v) &= \inf_{\rho\in X} \left(F_\lambda(\rho) + \langle v,\rho\rangle\right) \end{aligned} \tag{4}$$

- Moreau–Yosida regularisation

$$F_\lambda^\varepsilon(\rho) = \min_{\sigma\in X}\left(F_\lambda(\sigma) + \tfrac{1}{2\varepsilon}\|\sigma-\rho\|_X^2\right), \quad \varepsilon > 0 \tag{5}$$

- Proximal density

$$\rho^\varepsilon = \operatorname{prox}_{\varepsilon F}(\rho) = \operatorname*{argmin}_{\rho\in X}\left(F_\lambda(\sigma) + \tfrac{1}{2\varepsilon}\|\sigma-\rho\|_X^2\right) \tag{6}$$

Inversion Scheme

- Model functional

$$F^{\mathrm{mod}}_{\alpha,\xi}(\rho) = T_{\mathrm{s}}(\rho) + \alpha\langle v_{\mathrm{ext}}, \rho\rangle + \xi E_{\mathrm{H}}(\rho,\rho), \quad T_{\mathrm{s}}(\rho) = F_{\lambda=0}(\rho) \tag{7}$$

- Effective KS potential

$$v_s^{\varepsilon} = \alpha v_{\mathrm{ext}} + \xi v_{\mathrm{H}}(\rho^{\varepsilon}) + \boxed{\tfrac{1}{\varepsilon} J(\rho^{\varepsilon} - \rho_{\mathrm{ref}})}, \quad \rho^{\varepsilon} = \operatorname*{prox}_{\varepsilon F^{\mathrm{mod}}_{\alpha,\xi}}(\rho_{\mathrm{ref}}) \tag{8}$$

- Modified Hartee–Fock energy

$$\widetilde{\mathcal{E}}_{\mathsf{HF}}(D) = \mathrm{Tr}((T + \alpha v)D) + \lambda_{\mathrm{H}}\mathcal{E}_{\mathrm{H}}(D) - \lambda_{\mathrm{x}}\mathcal{E}_{\mathrm{x}}(D) + \tfrac{1}{2\varepsilon}\|\rho_D - \rho_{\mathrm{ref}}\|_X^2 \tag{9}$$

  - Forward: $\alpha = 1$, $v = v_{\mathrm{ext}}$, $\lambda_{\mathrm{H}} = \lambda_{\mathrm{x}} = 1$, and $1/\varepsilon = 0 \implies \rho_{\mathrm{ref}}$
  - Inverse: $\lambda_{\mathrm{x}} = 0$, $\lambda_{\mathrm{H}} = \xi$, and $v = v_{\mathrm{ext}} \implies v_{\mathrm{s}}$

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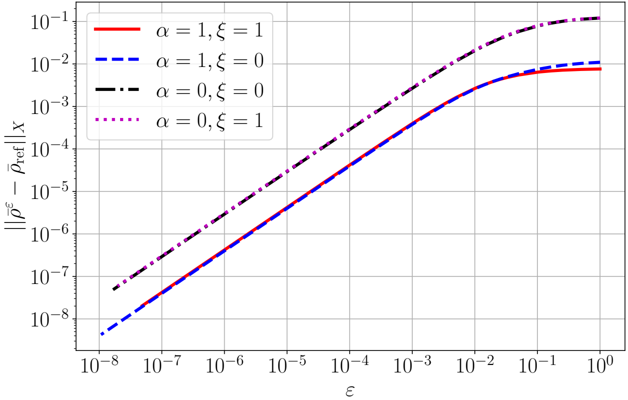
Results

Results

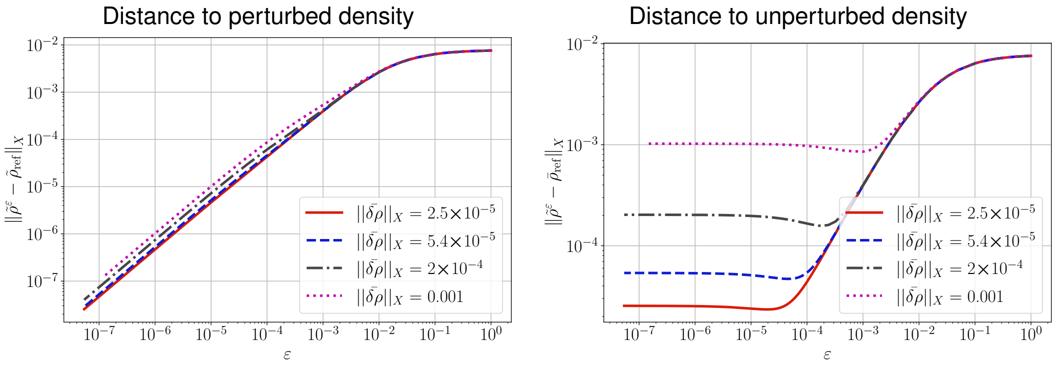
- 1D periodic Hartree–Fock model
- Exact exchange inversion
- Proof-of-principle for extended systems.



Error Analysis

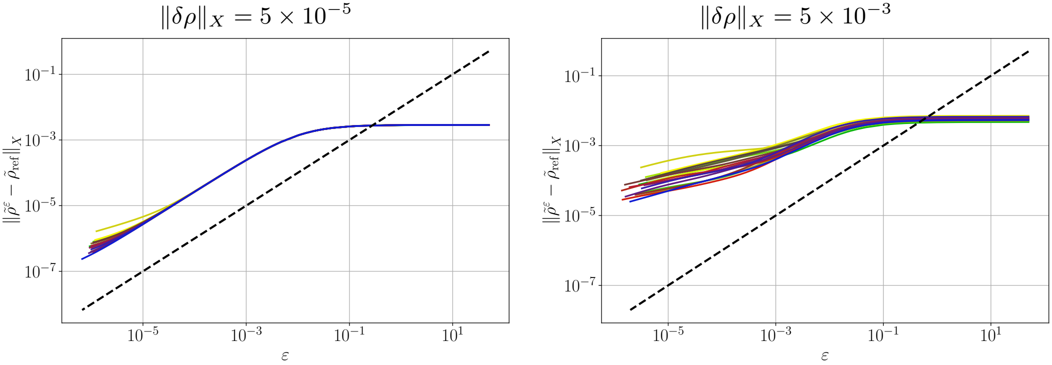
Fourier Mode Cut-Off

$$\widetilde{\rho}_{\text{ref}}(\mathbf{G}) = \rho_{\text{ref}}(\mathbf{G}) + \delta\rho(\mathbf{G}) = \begin{cases} \rho_{\text{ref}}(\mathbf{G}), & \text{if } |\mathbf{G}| \leq G_{\text{trunc}}, \\ 0, & \text{otherwise.} \end{cases} \tag{10}$$



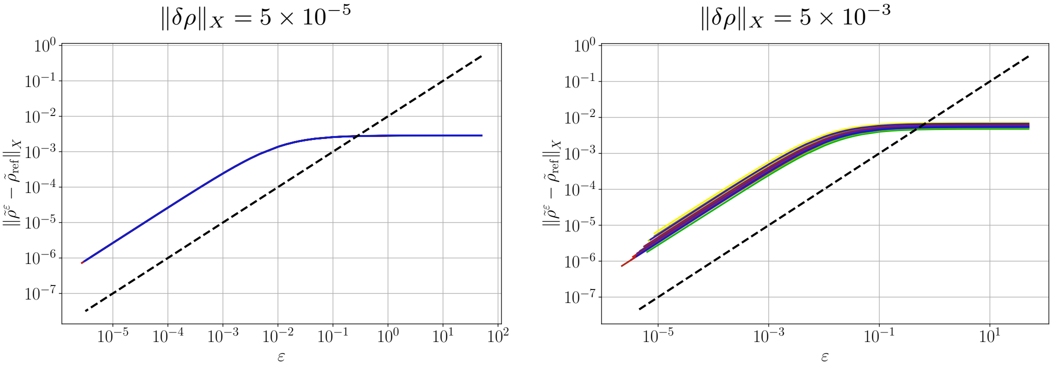
Normally Distributed Noise

- Perturbations $\delta\rho(\mathbf{G})$ drawn from $\mathcal{N}(0, \sigma_G)$
- Variance $\sigma_G^2 \propto G^{-2}$



Normally Distributed Noise

- More carefully selected noise model.



Outlook

Outlook

- Beyond exact exchange
- Higher-dimensional periodic systems

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- Improved exchange-correlation functional development

References

1. **Bohle, O. M. *et al.*** Regularized density-potential inversion for periodic systems: Application to exact exchange in one dimension. *The Journal of Chemical Physics* **164.** ISSN: 1089-7690. http://dx.doi.org/10.1063/5.0310171 (Feb. 2026).

Thank you!

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Inversion Scheme