Mathematical and Theoretical Aspects of Density-Functional Theory

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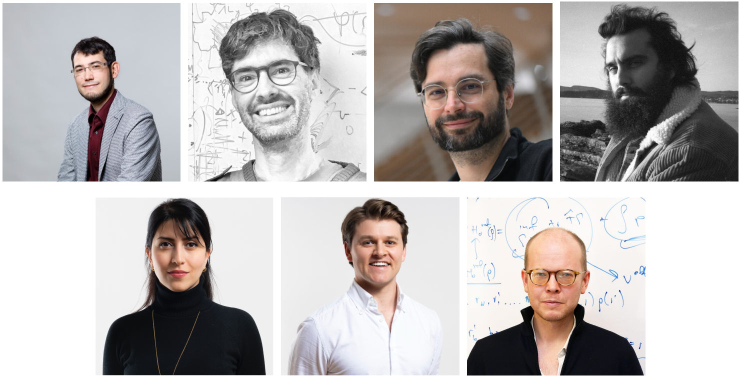

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Outline

1 Density-Functional Theory

2 QEDFT
- The Quantum Rabi Model
- A Hohenberg–Kohn Theorem
- The Universal Functional
- The Adiabatic Connection

3 Kohn–Sham Inversion
- The Periodic Setting
- Moreau–Yosida Regularisation
- The Inversion Algorithm
- A Numerical Example
- Error Bounds

4 Summary

Density-Functional Theory I

The N-body electronic Hamiltonian:

$$\widehat{H}^{\lambda}(v) = \widehat{T} + \lambda \widehat{W} + \widehat{V} \qquad\qquad \mathcal{H}_N = \bigwedge_{n=1}^{N} \mathcal{H}_1$$

$$\begin{aligned} E^{\lambda}(v) &= \inf_{|\psi\rangle \in \mathcal{W}_N} \langle \psi | \widehat{H}^{\lambda}(v) | \psi \rangle = \inf_{|\psi\rangle \in \mathcal{W}_N} \langle \psi | \widehat{T} + \lambda \widehat{W} + \widehat{V} | \psi \rangle \\ &= \inf_{\Gamma \in \mathcal{D}_N} \operatorname{Tr} \widehat{H}^{\lambda}(v) \Gamma \end{aligned}$$

$$\begin{aligned} \mathcal{W}_N &= \left\{ |\psi\rangle \in Q(\widehat{H}) \subset \mathcal{H}_N : \|\psi\| = 1,\ \langle \psi | \widehat{T} | \psi \rangle < +\infty \right\} \\ \mathcal{D}_N &= \left\{ \Gamma \in \mathfrak{S}_1(\mathcal{H}_N) : \widehat{T}\Gamma \in \mathfrak{S}_1(\mathcal{H}_N),\ \Gamma^{\dagger} = \Gamma \geq 0,\ \operatorname{Tr} \Gamma = 1 \right\} \end{aligned}$$

Density-Functional Theory II

$$\Gamma \longmapsto \rho \quad :\Longrightarrow \quad \rho(\mathbf{r}) = N \int \Gamma(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N; \mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N)\, \mathrm{d}\mathbf{r}_2 \dots \mathrm{d}\mathbf{r}_N$$

Recall: If $\Gamma \in \mathcal{D}_N$ is *pure*, then $\mathrm{Tr}\,\Gamma^2 = 1 \quad \Longleftrightarrow \quad \Gamma = |\psi\rangle\langle\psi|$ for $|\psi\rangle \in \mathcal{W}_N$

$$|\psi\rangle \longmapsto \rho \quad :\Longrightarrow \quad \rho(\mathbf{r}) = N \int |\psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N)|^2\, \mathrm{d}\mathbf{r}_2 \dots \mathrm{d}\mathbf{r}_N$$

Following Lieb[1]

$$\mathcal{I}_N = \left\{ \rho : \sqrt{\rho} \in H^1,\ \rho(\mathbf{r}) \geq 0, \int \rho(\mathbf{r})\, \mathrm{d}\mathbf{r} = N \right\} \subset L^1 \cap L^3$$

Any $\mathcal{I}_N \ni \rho \hookleftarrow |\psi\rangle \in \mathcal{W}_N$

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[1] Lieb, E. H. *Int. J. Quantum Chem.* **24**, 243–277 (1983).

Density-Functional Theory III

$$E^{\lambda}(v) = \inf_{\Gamma \in \mathcal{D}_N} \operatorname{Tr} \widehat{H}^{\lambda}(v)\Gamma = \inf_{\rho \in \mathcal{I}_N} \left\{ F_{\mathrm{L}}^{\lambda}(\rho) + \langle v,\, \rho \rangle \right\}$$

$$F_{\mathrm{L}}^{\lambda}(\rho) = \inf_{\Gamma \mapsto \rho} \operatorname{Tr}\left[(\widehat{T} + \lambda \widehat{W})\Gamma \right] \quad \longleftarrow \quad \text{mixed-state constrained-search functional}$$

$$F_{\mathrm{LL}}^{\lambda}(\rho) = \inf_{\Gamma \mapsto \rho} \langle \psi | \widehat{T} + \lambda \widehat{W} | \psi \rangle \quad \longleftarrow \quad \text{pure-state constrained-search functional}$$

$$F^{\lambda}(\rho) = \sup_{v \in X^*} \left\{ E^{\lambda}(v) - \langle v,\, \rho \rangle \right\} \quad \longleftarrow \quad \text{Legendre-Fenchel transform}$$

$$F^{\lambda}(\rho) \leq F_{\mathrm{L}}^{\lambda}(\rho) \leq F_{\mathrm{LL}}^{\lambda}(\rho) \qquad \forall \rho \in X$$

$$E^{\lambda}(v) = \inf_{\rho \in X} \left\{ F^{\lambda}(\rho) + \langle v,\, \rho \rangle \right\} = \inf_{\rho \in X} \left\{ F_{\mathrm{L}}^{\lambda}(\rho) + \langle v,\, \rho \rangle \right\} = \inf_{\rho \in X} \left\{ F_{\mathrm{LL}}^{\lambda}(\rho) + \langle v,\, \rho \rangle \right\}$$

Quantum Electrodynamical DFT

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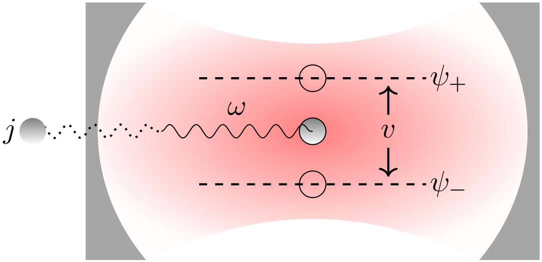
The Quantum Rabi Model

$$\mathcal{H} \simeq L^2(\mathbb{R}, \mathbb{C}^2)$$

$$\widehat{H}_0^\lambda = \frac{1}{2}\widehat{p}^2 + \frac{\omega^2}{2}\widehat{q}^2 + \lambda g \widehat{\sigma}_z \widehat{q} - t\widehat{\sigma}_x$$

$$\widehat{H}^\lambda(v,j) = \widehat{H}_0^\lambda + v\widehat{\sigma}_z + j\widehat{q}$$

$v \in \mathbb{R}$ $\quad$ $j \in \mathbb{R}$



$$\sigma := \langle \psi | \widehat{\sigma}_z | \psi \rangle \in [-1, 1]$$
$$\xi := \langle \psi | \widehat{q} | \psi \rangle \in \mathbb{R}$$

$$\widehat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \widehat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

“Density space”: $[-1, 1] \times \mathbb{R}$

Bakkestuen et al. *J. Phys. Chem. A* **129**, 2337–2360 (2025)

A Hohenberg–Kohn Theorem

Theorem (Weak HK)

Suppose that $|\psi_1\rangle, |\psi_2\rangle \in Q_0$ *are ground states of* $\widehat{H}(v_1, j_1)$ *and* $\widehat{H}(v_2, j_2)$*, respectively. If both* $|\psi_1\rangle, |\psi_2\rangle \mapsto (\sigma, \xi)$*, then* $|\psi_2\rangle$ *is a ground state of* $\widehat{H}(v_1, j_1)$ *and* $|\psi_1\rangle$ *is a ground state of* $\widehat{H}(v_2, j_2)$*.*

What about the usual formulation?

The density ρ uniquely determines the potential v up to an additive constant.

The Dicke Model

$$\widehat{H}_0^\lambda = \frac{1}{2}\widehat{p}^2 + \frac{\omega^2}{2}\widehat{q}^2 - \sum_{j=1}^{N} t_j \widehat{\sigma}_x^j + \sum_{j=1}^{N} \lambda g_j \widehat{q}\widehat{\sigma}_z^j, \qquad \widehat{\sigma}_a^j = \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes \underbrace{\widehat{\sigma}_a}_{j\text{th}} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1},$$

$$\boldsymbol{\sigma}_\psi = (\sigma_1, \ldots, \sigma_N)^\top, \qquad \sigma_j = \langle \psi | \widehat{\sigma}_z^j | \psi \rangle$$

Theorem (Strong HK)

Any $(\boldsymbol{\sigma}, \xi) \in \mathcal{R}_N \times \mathbb{R}$ *that is the density pair of a ground state uniquely determines an external pair* $(\mathbf{v}, j) \in \mathbb{R}^{N+1}$*. That is, the mapping*

$$\mathbb{R}^N \times \mathbb{R} \ni (\mathbf{v}, j) \longmapsto (\boldsymbol{\sigma}, \xi) \in \mathcal{R}_N \times \mathbb{R}$$

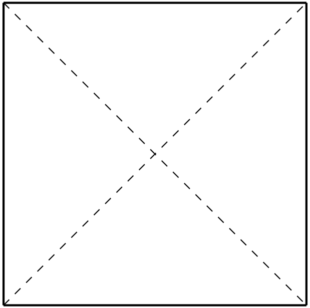
is an injection.

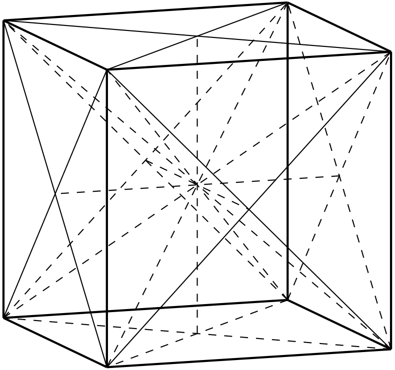
Regular Densities

A vector $\boldsymbol{\sigma} \in [-1,1]^N$ is *regular* if for every normalised $\chi \in \mathbb{R}_+^{2^N}$ with $\langle \chi | \widehat{\sigma}_z^j | \chi \rangle = \sigma_j$,

all $\{\chi, \widehat{\sigma}_z^1 \chi, \ldots, \widehat{\sigma}_z^N \chi\}$ are linearly independent.

$\mathcal{R}_N$: set of all regular $\boldsymbol{\sigma}$.





N-Representability

$$\mathcal{I}_N : (\sigma, \xi) \in [-1, 1] \times \mathbb{R}$$

Proof: pick $\psi(q) = \begin{pmatrix} \sqrt{1+\sigma} \\ \sqrt{1-\sigma} \end{pmatrix} \sqrt{\frac{\sqrt{\omega}}{2\sqrt{\pi}} e^{-\frac{\omega}{2}(q-\xi)^2}}$, then $\psi \mapsto (\sigma, \xi)$

Constraint manifold:

$$\mathcal{M}_{\sigma,\xi} = \{\psi \in Q_0 : \|\psi\| = 1,\ \sigma_\psi = \sigma,\ \xi_\psi = \xi\}.$$

The Constrained-Search Functional

$$E^\lambda(v,j) = \inf_{\psi \in Q_0} \langle \psi | \widehat{H}^\lambda(v,j) | \psi \rangle = \inf_{(\sigma,\xi)\in[-1,1]\times\mathbb{R}} \Big[F^\lambda_{\mathrm{LL}}(\sigma,\xi) + v\sigma + j\xi \Big]$$

$$F^\lambda_{\mathrm{LL}}(\sigma,\xi) = \inf_{\psi \in \mathcal{M}_{\sigma,\xi}} \langle \psi | \widehat{H}^\lambda_0 | \psi \rangle$$

Theorem

For every density pair $(\sigma,\xi) \in (-1,1) \times \mathbb{R}$ *there exists a unique real-valued and strictly positive optimizer* $|\psi\rangle \in \mathcal{M}_{\sigma,\xi}$ *of* $F_{\mathrm{LL}}(\sigma,\xi)$ *that is the (non-degenerate) ground-state solution of* $\widehat{H}^\lambda(v,j)\,|\psi\rangle = E^\lambda(v,j)\,|\psi\rangle$

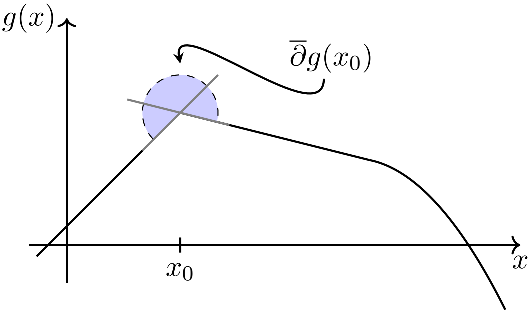
unique pure-state v-representability for $(\sigma,\xi) \in (-1,1) \times \mathbb{R}$

$$F^\lambda_{\mathrm{LL}}(\sigma,\xi) = F^\lambda_{\mathrm{L}}(\sigma,\xi) = F^\lambda(\sigma,\xi) \qquad \forall (\sigma,\xi) \in (-1,1) \times \mathbb{R}$$

Superdifferentiability

Let $g : X \to \mathbb{R} \cup \{-\infty\}$ be a proper, concave, and upper semicontinuous functional

$$\overline{\partial} g(x) = \{x^* \in X^* : g(x) + \langle x^*, y - x\rangle \geq g(y), \forall y \in X\}$$



$$\rho \in \overline{\partial} E(v)$$

if $f(x) = -g(x)$, $\underline{\partial} f(x) = -\overline{\partial} g(x)$.

$$-v \in \overline{\partial} F(\rho)$$

A Generalised Newton–Leibniz Formula

Let $g : \mathbb{R} \to \mathbb{R}$.
Suppose that $[a, b]$ is contained in the interior of $\operatorname{dom} g$.
Then for any $\mathfrak{g}(x) \in \overline{\partial} g(x)$,

$$g(b) = g(a) + \int_a^b \mathfrak{g}(x) \, \mathrm{d}x \, .$$

The Adiabatic Connection Functional

$$g\,\langle\psi^\lambda|\widehat{\sigma}_z\widehat{q}|\psi^\lambda\rangle \in \overline{\partial}_\lambda F^\lambda(\sigma,\xi)$$

$$\begin{aligned}
F^\lambda(\sigma,\xi) &= \overbrace{\frac{\omega}{2} - t\sqrt{1-\sigma^2} + \frac{\omega^2}{2}\xi^2}^{F^0(\sigma,\xi)} + \int_0^\lambda g\,\langle\psi^\mu|\widehat{\sigma}_z\widehat{q}|\psi^\mu\rangle\,\mathrm{d}\mu \\
&= \frac{\omega}{2} - t\sqrt{1-\sigma^2} + \frac{\omega^2}{2}\xi^2 + \underbrace{\lambda g\sigma\xi}_{D(\sigma,\xi)} - \frac{\lambda^2 g^2}{2\omega^2}(1-\sigma^2) - \frac{4t}{\omega^2}\int_0^\lambda\int_{\mathbb{R}} \varphi_+^{\mu\,\prime}\varphi_-^\mu\,\mathrm{d}q\,\mathrm{d}\mu
\end{aligned}$$

$\varphi_\pm^\lambda(q)$ the optimisers of $F^\lambda(\sigma,0)$

Standard DFT:

$$F^\lambda(\rho) = T(\rho) + \lambda E_{\mathrm{H}}(\rho) + \int_0^\lambda \Big(\mathrm{Tr}\Big[\widehat{W}\Gamma^\mu\Big] - E_{\mathrm{H}}(\rho)\Big)\,\mathrm{d}\mu$$

Correlation Energy in QRabi

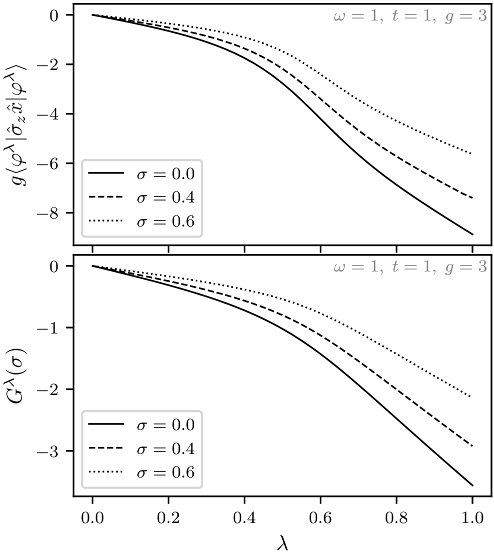
$$\lambda E_{\mathrm{c}}^{\lambda}(\sigma,\xi) = F^{\lambda}(\sigma,\xi) - F^{0}(\sigma,\xi) - \lambda D(\sigma,\xi)$$

$$E_{\mathrm{c}}^{\lambda}(\sigma,\xi) = -\lambda\frac{g^2}{2\omega^2}\left(1-\sigma^2\right) + I^{\lambda}(\sigma)$$

$$I^{\lambda}(\sigma) := -\frac{4tg}{\omega^2}\int_0^{\lambda}\int \varphi_+^{\mu\,\prime}\varphi_-^{\mu}\,\mathrm{d}q\,\mathrm{d}\mu\,.$$

Conjecture in standard DFT [3]:

$\overline{\partial}_{\lambda}F^{\lambda}(\rho) - E_{\mathrm{H}}(\rho) \ni f^{\lambda}(\rho)$ $\longleftarrow$ convex in λ

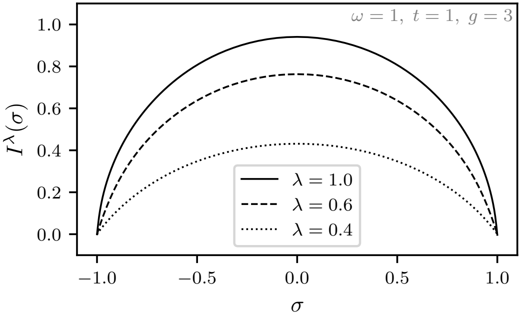


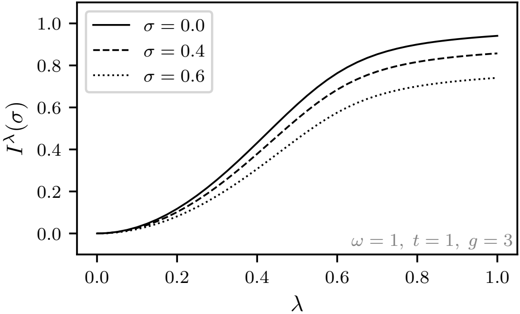
Non-Explicit Correlation

$$0 \leq I^\lambda(\sigma) \leq \frac{\lambda^2 g^2}{2\omega^2}(1-\sigma^2).$$

Conjecture:

$$I^\lambda(\sigma) = \omega \frac{b(\lambda,t)}{a(\lambda,t)} \left[\sqrt{a(\lambda,t)^2-\sigma^2} \right. \\ \left. -\sqrt{a(\lambda,t)^2-1}\right]$$





Kohn–Sham Inversion

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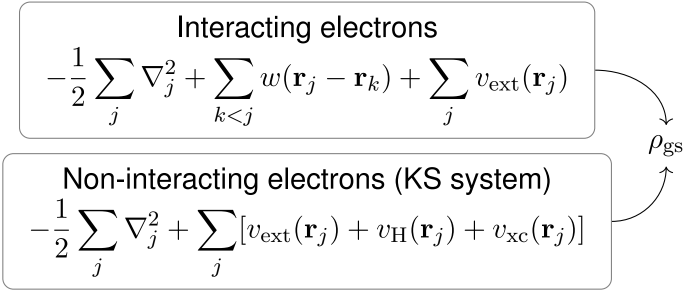
The Inverse Kohn–Sham Problem



Interacting electrons

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

Non-interacting electrons (KS system)

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

ρ_{gs}

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

The Periodic Setting

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

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

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)

Moreau–Yosida Regularisation

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

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

Unique optimiser: *the proximal point*

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

The Guiding Functional

Goal: Given ρ_{gs}, determine v_{xc}

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

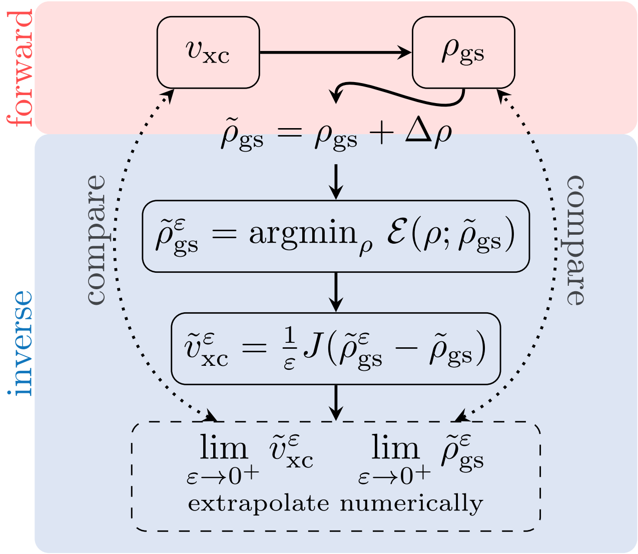
Minimise $$\mathcal{E}(\rho;\rho_{\mathrm{gs}}) = \mathcal{F}(\rho) + \frac{1}{2\varepsilon}\|\rho - \rho_{\mathrm{gs}}\|_{\mathcal{X}}^{2}$$

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

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

Penz et al. *Electron. Struct.* **5**, 014009 (2023)
Herbst, Bakkestuen, Laestadius *Phys. Rev. B* **111**, 205143 (2025)
Bakkestuen *et al.* In preparation (2026)

The Inversion Algorithm



$$v_{\mathrm{xc}} \longrightarrow \rho_{\mathrm{gs}}$$

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

$$\tilde{\rho}_{\mathrm{gs}}^{\varepsilon} = \operatorname{argmin}_{\rho}\ \mathcal{E}(\rho;\tilde{\rho}_{\mathrm{gs}})$$

$$\tilde{v}_{\mathrm{xc}}^{\varepsilon} = \frac{1}{\varepsilon} J(\tilde{\rho}_{\mathrm{gs}}^{\varepsilon} - \tilde{\rho}_{\mathrm{gs}})$$

$$\lim_{\varepsilon\to 0^+} \tilde{v}_{\mathrm{xc}}^{\varepsilon} \qquad \lim_{\varepsilon\to 0^+} \tilde{\rho}_{\mathrm{gs}}^{\varepsilon}$$

extrapolate numerically

Planewave KS-DFT:

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

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

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

DFTK

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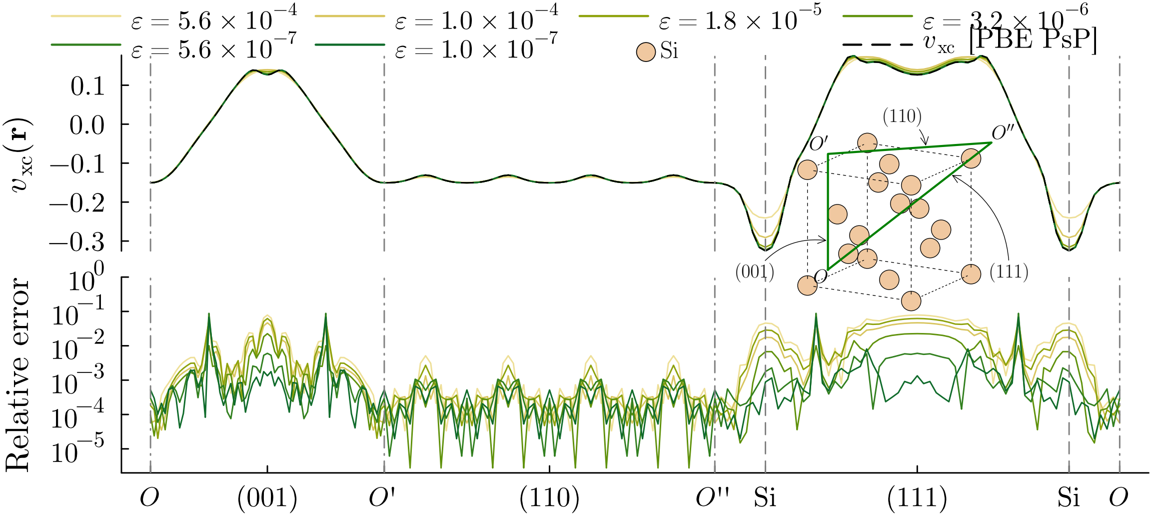
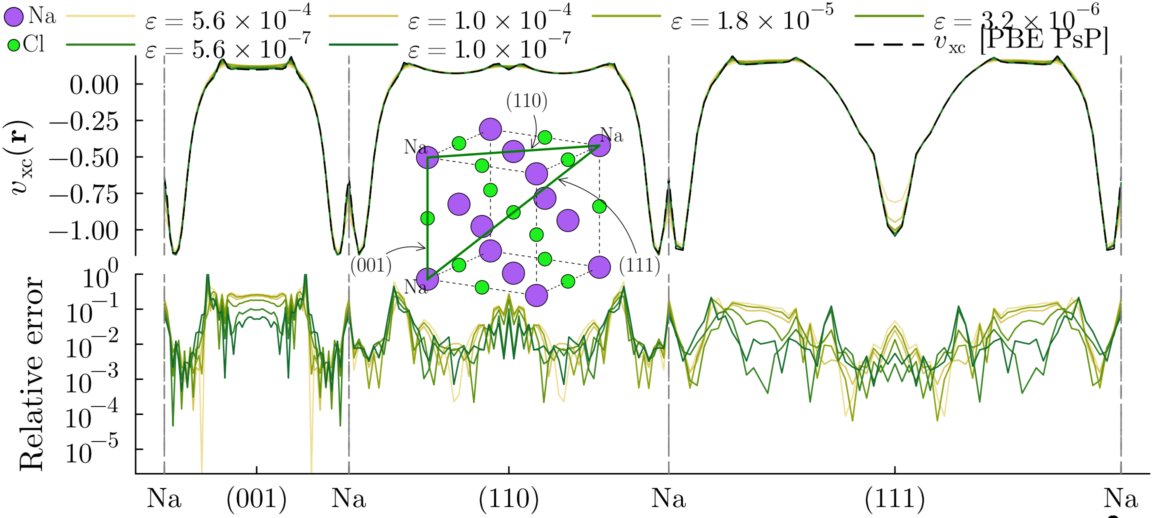
Bulk Silicon

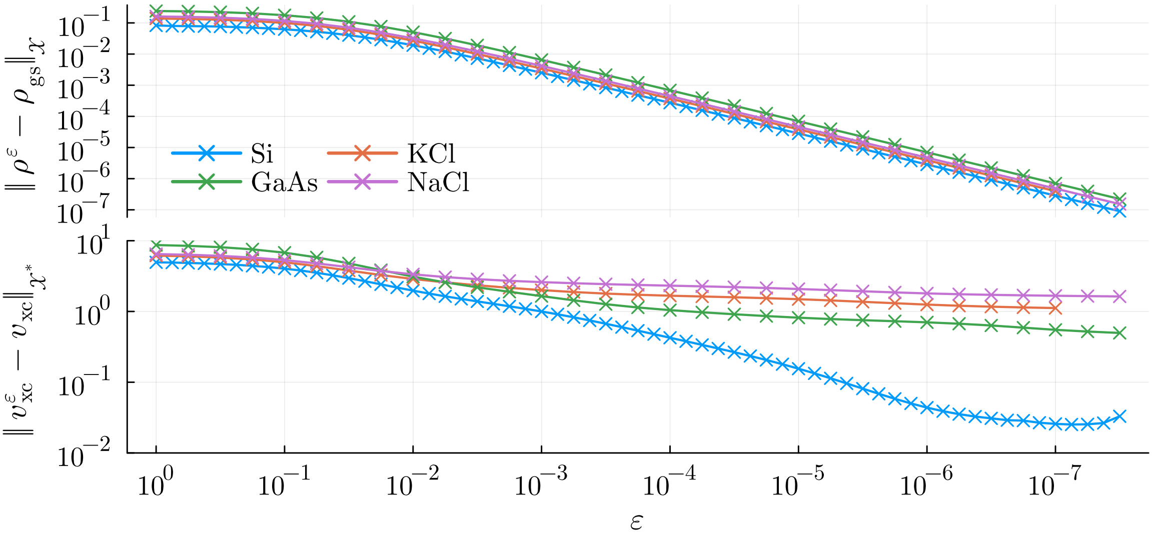


Implementation: `github.com/vebjorhb/MY-periodic-inversion`

Sodium Chloride



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*

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

Herbst, Bakkestuen, Laestadius *Phys. Rev. B* **111**, 205143 (2025)
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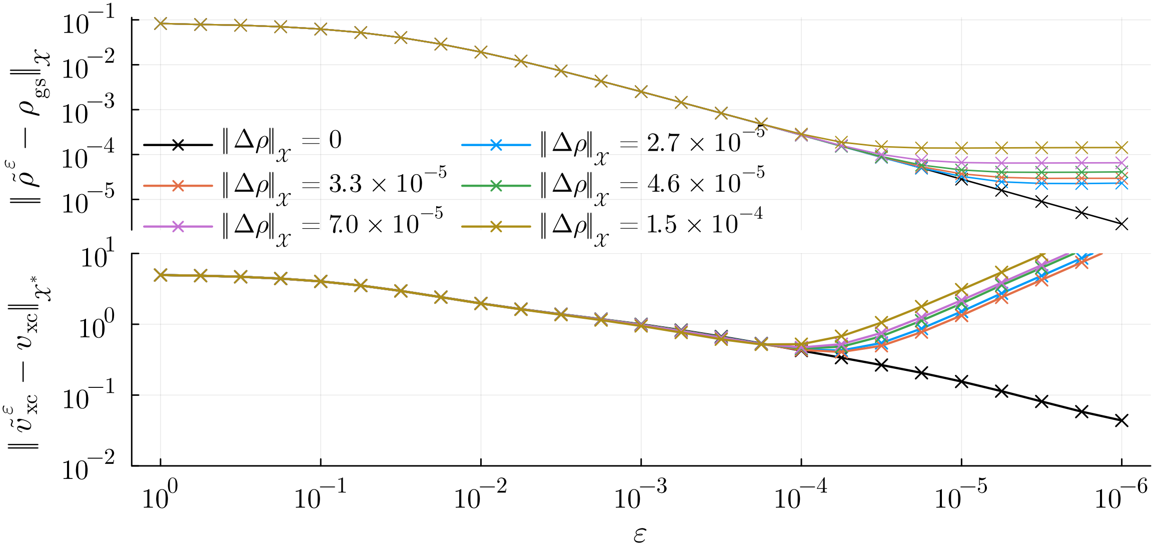
Bulk Silicon



Summary

QEDFT for the Quantum Rabi model

- Almost explicit DFT
- Illustrates central ideas in DFT without approximations

Kohn–Sham Inversion

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

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Thank you for your attention!

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