Moreau–Yosida Density-Potential Inversion

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Acknowledgements

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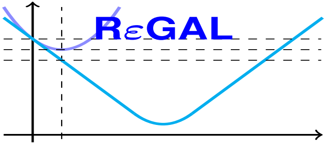
Funded under ERC StG No. 101041487 REGAL



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Established by the European Commission

Outline

Introduction

- **Challenge**: No explicit formula exists for total energy from electron density in many-body quantum systems.
- **Kohn-Sham (KS) Method**: Approximates energy using an exchange-correlation (xc) functional.
- **Objective**: Derive effective potentials from densities via variational principles and optimization (e.g., MY regularization).

Interacting electrons

$$\widehat{H} = -\frac{1}{2}\sum_j \nabla_j^2 + \sum_{k<j} |\mathbf{r}_j - \mathbf{r}_k|^{-1} + \sum_j v_{\mathrm{ext}}(\mathbf{r}_j) \longrightarrow \rho_{\mathrm{gs}}$$

Non-interacting electrons (KS system)

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

Mathematical Framework

- **Functional** $\mathcal{F}(\rho)$:
  - Represents the internal energy of a non-interacting system as a function of the density ρ.
  - $\mathcal{F}(\rho)$ is convex and lower semicontinuous (lsc).
- **Space** $\mathcal{D}$:
  - $\mathcal{D}$ is a Banach space, assumed to be uniformly convex.
  - The density ρ belongs to this space: $\rho \in \mathcal{D}$.
- **Duality Mapping** $\mathcal{J}$:
  - $\mathcal{J} : \mathcal{D} \to \mathcal{D}^*$ is defined by:

$$\mathcal{J}(\rho) = \left\{ v \in \mathcal{D}^* : \|v\|^2_{\mathcal{D}^*} = \|\rho\|^2_{\mathcal{D}} = \langle v, \rho \rangle \right\} \quad \Rightarrow \quad \mathcal{J}(\rho) = \underline{\partial}(\frac{1}{2}\|\rho\|^2_{\mathcal{D}})$$

  - Associates each $\rho \in \mathcal{D}$ with $v \in \mathcal{D}^*$ satisfying the above conditions.
  - In uniformly convex spaces, $\mathcal{J}$ is single-valued and captures the dual relationship between densities and potentials.

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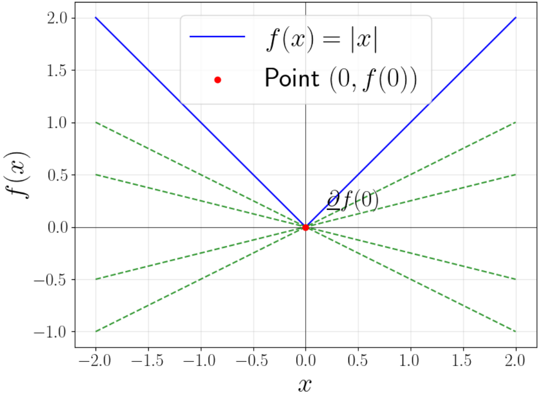
The Subdifferential $\underline{\partial}$

- Differentiability cannot always be assumed, especially for convex functionals on infinite-dimensional spaces.
- **Subdifferential $\underline{\partial}$** generalizes the gradient concept:

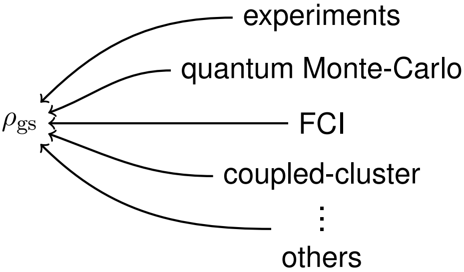
$$\underline{\partial} f(\rho) = \{v \in X^* \mid f(\rho') - f(\rho) \geq \langle v, \rho' - \rho \rangle, \quad \forall \rho' \in X\} \tag{1}$$



Kohn-Sham Inversion

Kohn-Sham Inversion

- **Kohn-Sham (KS) Inversion**: Reconstructs energy functional from ground-state density by finding the corresponding potential.
- Enables development of accurate xc functionals.



Moreau-Yosida Regularization

Moreau-Yosida Regularization

- **Moreau-Yosida (MY) Regularization**: Handles stability and non-differentiability in optimization.
- Combines regularization with optimization to derive accurate potentials.

Definition

Let $\mathcal{D}$ be uniformly convex and $\mathcal{F} : \mathcal{D} \to \mathbb{R}$ convex and lower semicontinuous functional. For some $\varepsilon > 0$, the *Moreau-Yosida regularization* of $\mathcal{F}$ at ρ_{gs} is

$$\mathcal{F}^{\varepsilon}(\rho_{\mathsf{gs}}) = \inf_{\rho \in \mathcal{D}} \left\{ \mathcal{F}(\rho) + \frac{1}{2\varepsilon} \left\| \rho - \rho_{\mathsf{gs}} \right\|_{\mathcal{D}}^{2} \right\}.$$

Variational Formulation of the Problem

- **Optimization Problem**:

$$\min_{\rho\in\mathcal{D}} \left(\underbrace{\mathcal{F}(\rho) + \frac{1}{2\varepsilon}\|\rho - \rho_{\mathrm{gs}}\|_{\mathcal{D}}^2}_{\mathcal{E}(\rho\,;\rho_{\mathrm{gs}})} \right) \tag{2}$$

- The regularization term keeps ρ close to the reference density ρ_{gs}, with $\varepsilon > 0$ controlling the penalty's strength.
- The proximal point $\rho^\varepsilon = \operatorname{argmin}_{\rho\in\mathcal{D}} \mathcal{E}(\rho, \rho_{\mathrm{gs}})$ minimizes this expression.
- The stationary condition for this optimization is:

$$\underline{\partial}\mathcal{F}(\rho^\varepsilon) + \frac{1}{\varepsilon} J(\rho^\varepsilon - \rho_{\text{gs}}) \ni 0.$$

Derivation of V_{eff}

- The ground-state density ρ_{gs} is defined as:

$$\rho_{\text{gs}} = \underset{\rho \in \mathcal{D}}{\operatorname{argmin}} \left(\mathcal{F}(\rho) + \langle V_{\text{eff}}, \rho \rangle \right)$$

- The proximal point $\rho^{\varepsilon}(\rho_{\text{gs}})$ is defined as:

$$\rho^{\varepsilon}(\rho_{\text{gs}}) = \underset{\rho \in \mathcal{D}}{\operatorname{argmin}} \left(\mathcal{F}(\rho) + \frac{1}{2\varepsilon} \|\rho - \rho_{\text{gs}}\|_{\mathcal{D}}^{2} \right)$$

- The stationary condition leads to:

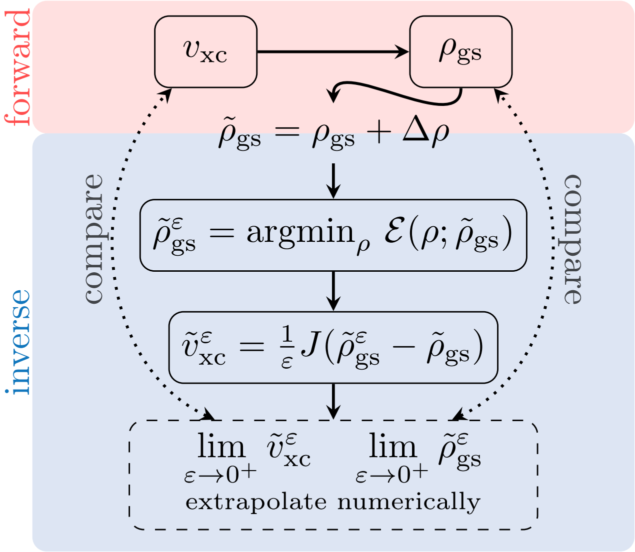
$$\underline{\partial} \mathcal{F}(\rho_{\text{gs}}) + V_{\text{eff}} \ni 0$$

$$\underline{\partial} \mathcal{F}(\rho^{\varepsilon}) + \frac{1}{\varepsilon} J(\rho^{\varepsilon} - \rho_{\text{gs}}) \ni 0$$

- As $\varepsilon \to 0$ and $\rho^{\varepsilon} \to \rho_{\text{gs}}$, the effective potential V_{eff} is derived as:

$$V_{\text{eff}} = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} J(\rho^{\varepsilon} - \rho_{\text{gs}})$$

The Inversion Algorithm



Example: Regularization of a Simple Function

- Let $\rho \in \mathbb{R}$. Consider the functional:

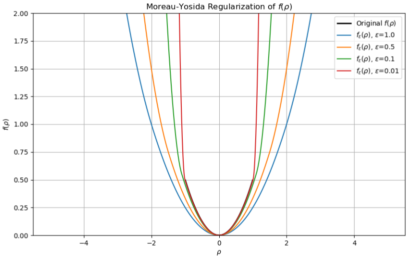
$$\mathcal{F}(\rho) = \begin{cases} \frac{1}{2}\rho^2, & \text{if } |\rho| \leq 1, \\ \infty, & \text{if } |\rho| > 1 \end{cases}$$

- MY regularization smooths the non-differentiable edge at $|\rho| = 1$.

Example: Regularization of a Simple Function

- The original and regularized functionals are:

$$\mathcal{F}(\rho) = \begin{cases} \frac{1}{2}\rho^2, & \text{if } |\rho| \leq 1, \\ \infty, & \text{if } |\rho| > 1 \end{cases} \quad \Rightarrow \quad \mathcal{F}^{\varepsilon}(\rho) = \begin{cases} \frac{1}{2} + \frac{1}{2\varepsilon}(1-\rho)^2, & \text{if } \rho \geq 1+\varepsilon, \\ \frac{\rho^2}{2(1+\varepsilon)}, & \text{if } |\rho| \leq 1+\varepsilon, \\ \frac{1}{2} + \frac{1}{2\varepsilon}(1+\rho)^2, & \text{if } \rho \leq -1-\varepsilon. \end{cases}$$



Example: Regularization of a Simple Function

- The solution ρ_ε is given by:

$$\rho^\varepsilon = \begin{cases} -1 & \text{if } \rho \leq -1-\varepsilon \\ \frac{\rho}{\varepsilon+1} & \text{if } |\rho| \leq 1+\varepsilon \\ 1 & \text{if } \rho \geq 1+\varepsilon \end{cases}$$

- Within the interval $|\rho| \leq 1+\varepsilon$,

$$|\rho^\varepsilon(\rho_1) - \rho^\varepsilon(\rho_2)| = \frac{1}{1+\varepsilon} |\rho_1 - \rho_2|, \quad \forall \rho_1, \rho_2 \in [-1-\varepsilon, 1+\varepsilon].$$

Since $\frac{1}{1+\varepsilon} < 1$ for $\varepsilon > 0$, the proximal map ρ^ε is indeed a contraction mapping.

Example: Regularization of a Simple Function

For $\rho_{\text{gs}} \in (-1, 1)$, the proximal map $\rho^{\varepsilon} = \frac{\rho_{\text{gs}}}{1+\varepsilon}$.
The duality mapping J in this case is trivial ($J(x) = x$), so:

$$\frac{1}{\varepsilon} J(\rho^{\varepsilon} - \rho_{\text{gs}}) = \frac{1}{\varepsilon}\left(-\frac{\varepsilon \rho_{\text{gs}}}{1+\varepsilon}\right) = -\frac{\rho_{\text{gs}}}{1+\varepsilon}.$$

Taking the limit as $\varepsilon \to 0$:

$$V_{\text{eff}} = \lim_{\varepsilon \to 0} -\frac{\rho_{\text{gs}}}{1+\varepsilon} = -\rho_{\text{gs}}.$$

Thus, the effective potential is:

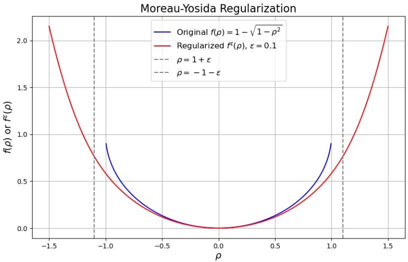
$$V_{\text{eff}} = -\rho_{\text{gs}}, \quad \rho_{\text{gs}} \in (-1, 1).$$

Numerical Example

- Consider the functional:

$$\mathcal{F}(\rho) = \begin{cases} 1 - \sqrt{1-\rho^2}, & \text{if } |\rho| \leq 1, \\ \infty, & \text{if } |\rho| > 1 \end{cases}$$

- Apply MY regularization for $\varepsilon = 0.1$.
- The regularized functional $\mathcal{F}^\varepsilon(\rho)$ becomes smoother, eliminating non-differentiable points.



Summary

- **Objective:** Reconstruct effective potentials V_{eff} from given densities using variational principles and Moreau-Yosida (MY) regularization.
- **Kohn-Sham Inversion:** Links ground-state density ρ_{gs} to effective potentials for more accurate xc functionals.
- **MY Regularization:**
  - Smooths non-differentiabilities in optimization problems.
  - Ensures stability and convergence through the proximal map.
- **Effective Potential:**

$$V_{\text{eff}} = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} J(\rho^{\varepsilon} - \rho_{\text{gs}})$$

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Thank you for your attention!
Questions?

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Non-Expansive Property of the Proximal Map

- **Proximal Map**:

$$\rho^{\varepsilon} = \operatorname{prox}_{\varepsilon f}(\rho)$$

- **Non-Expansive Property**:

$$\|\rho_1^{\varepsilon} - \rho_2^{\varepsilon}\| \leq \|\rho_1 - \rho_2\|, \quad \forall \rho_1, \rho_2 \in \mathcal{D}$$

- The mapping $\rho \mapsto \rho^{\varepsilon}(\rho)$ is non-expansive for each $\varepsilon > 0$.
- This property ensures stability in optimization and guarantees convergence of iterative schemes using the proximal map.