Uniqueness, regularity, compactness and inversion of the potential-to-density map $v \mapsto \rho(v)$ of quantum mechanics

Louis Garrigue

September 15, 2020

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- Density functional theory (DFT) is the most efficient method to probe matter at microscopic scale (five to hundreds of electrons)
- Very few mathematical works on the foundations of DFT

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- To have $\langle \Psi, H(v)\Psi \rangle \geqslant -c \langle \Psi, \Psi \rangle$, need $v \in (L^p + L^\infty)(\mathbb{R}^d, \mathbb{R})$ with

$$\begin{cases} p = 1 & \text{for } d = 1 \\ p > 1 & \text{for } d = 2 \\ p = d/2 & \text{for } d \geqslant 3. \end{cases}$$

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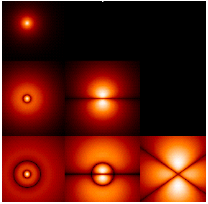
- n^{th} excited state φ_n is given by $\inf_{\substack{\int |\Psi|^2 = 1 \\ \Psi \perp \mathrm{Span}(\varphi_0, \ldots, \varphi_{n-1})}} \langle \Psi, H(v)\Psi \rangle$



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- One-body density $\rho \in L^1(\mathbb{R}^d, \mathbb{R}_+)$, experimentally measurable

$$\rho_\Psi(x) := N \int_{\mathbb{R}^{d(N-1)}} |\Psi|^2 (x, x_2, \ldots, x_N) \mathrm{d}x_2 \cdots \mathrm{d}x_N$$

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$$W(\Psi) := \sum_{i<j} \int_{\mathbb{R}^{dN}} w(x_i - x_j) |\Psi|^2 (x_1, \dots, x_N) \mathrm{d}x_1 \cdots \mathrm{d}x_N$$

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- Curse of dimensionality
- If $w = 0$, then $\Psi = \wedge_{i=0}^{N-1} \varphi_i$ where φ_i are the first eigenstates of $-\Delta + v$, $E^N(v) = \sum_{i=0}^{N-1} \left(\int_{\mathbb{R}^d} |\nabla \varphi_i|^2 + \int_{\mathbb{R}^d} v\, |\varphi_i|^2 \right)$, and $\rho_\Psi = \sum_{i=0}^{N-1} |\varphi_i|^2$

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  Main goal of DFT : express everything in terms of ρ
- Kohn-Sham (1965) : replace (v, w) by v_{ks} such that
  $\boxed{\rho_{w=0}(v_{ks}) = \rho(v)}$ where $\rho_{w=0}(v_{ks})$ is the ground state density of

$$H^N_{w=0}(v) = \sum_{i=1}^{N} \left(-\Delta_{x_i} + v_{\text{ks}}(x_i) \right)$$

Kohn-Sham orbitals φ_i, $\Psi_{\text{ks}} = \wedge_{i=0}^{N-1} \varphi_i$, $\sum_{i=0}^{N-1} |\varphi_i|^2 = \rho(v)$

ρ contains everything

- Thomas-Fermi theory for $w = |\cdot|^{-1}$ (1927)

$$E^N(\rho) \simeq c_{\mathrm{TF}} \int_{\mathbb{R}^3} \rho^{5/3} + \frac{1}{2} \int_{\mathbb{R}^6} \frac{\rho(x)\rho(y)}{|x-y|} \mathrm{d}x\mathrm{d}y + \int_{\mathbb{R}^3} v\rho$$

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- Hohenberg-Kohn theorem (1964)
- Universal Levy-Lieb functional (1984), for $\rho \in L^1(\mathbb{R}^d)$ such that $\sqrt{\rho} \in H^1$ and $\int \rho = N$,

$$F(\rho) := \inf_{\substack{\Psi \in H^1(\mathbb{R}^{dN}) \\ \int |\Psi|^2 = 1 \\ \rho_\Psi = \rho}} \left(\int_{\mathbb{R}^{dN}} |\nabla \Psi|^2 + W(\Psi) \right)$$

$$E^N(v) = \inf_{\substack{\rho \in L^1(\mathbb{R}^d) \\ \int \rho = N \\ \sqrt{\rho} \in H^1}} \left(F(\rho) + \int_{\mathbb{R}^d} v\rho \right)$$

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- Approximate $F(\rho)$: "graal" of DFT

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- Lieb-Thirring (1976)

$$c_{\rm LT} \int_{\mathbb{R}^d} \rho_\Psi^{1+\frac{2}{d}} \leqslant \int_{\mathbb{R}^{dN}} |\nabla \Psi|^2$$

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- Uniform electrons gaz in Lewin-Lieb-Seiringer (2018, 2019), jellium to Dirac order by Lieb-Narnhofer (1975), Graf-Solovej (1994), next order by Hainzl-Porta-Rexze (2020) and Benedikter-Nam-Porta-Schlein-Seiringer (2020)

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   - The set of binding potentials
   - Regularity and weak-strong continuity of $v \mapsto \Psi(v)$
   - Degenerate potentials
3. The Kohn-Sham problem
   - Regularization of the problem
   - Numerical inversion

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Hohenberg-Kohn theorem

$$H^N(v) := \sum_{i=1}^{N} -\Delta_i + \sum_{1\leqslant i<j\leqslant N} w(x_i - x_j) + \sum_{i=1}^{N} v(x_i)$$

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Theorem (Hohenberg-Kohn)

Let $w, v_1, v_2 \in$?. If there are two ground states Ψ_1 and Ψ_2 of $H^N(v_1)$ and $H^N(v_2)$, such that

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- We can take **?** $= L^{\frac{dN}{2}}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ by Jerison-Kenig (1985)

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4. Using $\int_{\mathbb{R}^d}(v_1 - v_2)(\rho_{\Psi_1} - \rho_{\Psi_2}) = 0$, the $\leqslant$'s above are $=$, hence $\langle \Psi_2, H^N(v_1)\Psi_2 \rangle = E_1$, that is Ψ_2 is a ground state for $H^N(v_1)$, so $H^N(v_1)\Psi_2 = E_1\Psi_2$

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5. Substracting it with $H^N(v_2)\Psi_2 = E_2\Psi_2$, we get

$$\left(E_1 - E_2 + \sum_{i=1}^N (v_2 - v_1)(x_i)\right) \Psi_2 = 0$$

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1. $\left\langle \Psi, \left(\sum_{i=1}^{N} v(x_i)\right) \Psi \right\rangle = \int_{\mathbb{R}^d} v \rho_\Psi$
2. $E_1 \leqslant \langle \Psi_2, H^N(v_1)\Psi_2 \rangle = E_2 + \int_{\mathbb{R}^d} \rho_{\Psi_2}(v_1 - v_2)$
3. Exchanging $1 \leftrightarrow 2$ gives $E_1 - E_2 \geqslant \int_{\mathbb{R}^d} \rho_{\Psi_1}(v_1 - v_2)$
4. Using $\int_{\mathbb{R}^d}(v_1 - v_2)(\rho_{\Psi_1} - \rho_{\Psi_2}) = 0$, the $\leqslant$'s above are $=$, hence $\langle \Psi_2, H^N(v_1)\Psi_2 \rangle = E_1$, that is Ψ_2 is a ground state for $H^N(v_1)$, so $H^N(v_1)\Psi_2 = E_1\Psi_2$
5. Substracting it with $H^N(v_2)\Psi_2 = E_2\Psi_2$, we get

$$\left(E_1 - E_2 + \sum_{i=1}^{N}(v_2 - v_1)(x_i)\right) \Psi_2 = 0$$

6. By strong unique continuation, $|\{\Psi_2(X) = 0\}| = 0$, thus $E_1 - E_2 + \sum_{i=1}^{N}(v_2 - v_1)(x_i) = 0$ and integrating on $[0, L]^{d(N-1)}$, we obtain $v_1 = v_2 + (E_1 - E_2)/N$

Strong UCP

Theorem (Strong UCP for many-body Schrödinger operators)

Assume that the potentials satisfy

$$v, w \in L^p_{\mathrm{loc}}(\mathbb{R}^d) \qquad \text{with } p > \max\left(2d/3, 2\right).$$

If $\Psi \in H^2_{\mathrm{loc}}(\mathbb{R}^{dN})$ *is a non zero solution to* $H^N(v)\Psi = E\Psi$*,*
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- In $3D$, we can take **?** $= L^{p>2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Covers Coulomb-like singularities

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- Works for excited states

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Magnetic case, the Pauli Hamiltonian

$$H^N(v,A) := \sum_{j=1}^{N} \Big(\big(\sigma_j \cdot (-i\nabla_j + A(x_j))\big)^2 + v(x_j) \Big) + \sum_{1\leqslant i<j\leqslant N} w(x_i - x_j)$$

Theorem (Strong UCP for the many-body Pauli operator)

Assume that the potentials satisfy $\operatorname{div} A = 0$ *and*

$$\begin{aligned} A &\in L^q_{\rm loc}(\mathbb{R}^d) &\qquad \text{with } q > 2d, \\ \operatorname{curl} A, v, w &\in L^p_{\rm loc}(\mathbb{R}^d) &\qquad \text{with } p > \max\left(2d/3, 2\right). \end{aligned}$$

If $\Psi \in H^2_{\rm loc}(\mathbb{R}^{dN})$ *is a non zero solution to* $H^N(v,A)\Psi = E\Psi$, *then* $|\{\Psi(X) = 0\}| = 0$.

History of related UCP results

	Date	Weak or Strong	Number of particles	Hypothesis on v (loc)	Magnetic ?
Carleman	39	W	1 (and N)	L^∞	No
Hörmander	63	W	1	$L^{2d/3}$	No
Georgescu	80	W	N	$L^{2d/3}$	No
Schechter-Simon	80	W	N	L^d	No
Jerison-Kenig	85	S	1	$L^{d/2}$	No
Kurata	97	S	1	Many	Yes
Koch-Tataru	01	S	1	$L^{d/2}$	Yes
Laestadius-Benedicks-Penz	18	S	N	Many	Yes
Garrigue	19	S	N	$L^{p>2d/3}$	Yes

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Other works : Kinzebulatov-Shartser (2010), Lammert (2018)

Carleman-type inequality

De Figueiredo-Gossez (1992) : if $|\{\Psi(X) = 0\}| > 0$, then $\int \frac{|\Psi|^2}{|X - X_0|^\tau}$ is finite for all τ. Take $X_0 = 0$.

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Theorem (Carleman-type inequality)

Define $\phi(X) := (-\ln|X|)^{-1/2}$. *We have*

$$\tau^3 \int_{B_{1/2}} \phi^5 \left|\frac{e^{(\tau+2)\phi}\Psi}{|X|^{\tau+2}}\right|^2 + \tau \int_{B_{1/2}} \phi^5 \left|\nabla\left(\frac{e^{(\tau+1)\phi}\Psi}{|X|^{\tau+1}}\right)\right|^2 + \tau^{-1}\int_{B_{1/2}} \phi^5 \left|\Delta\left(\frac{e^{\tau\phi}\Psi}{|X|^{\tau}}\right)\right|^2 \leqslant c\int_{B_{1/2}} \left|\frac{e^{\tau\phi}\Delta\Psi}{|X|^{\tau}}\right|^2 .$$

Fractional Carleman

- With Hardy's inequality $|X|^{-2s} \leqslant (-\Delta)^s$, it transforms into

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Corollary (Carleman fractionnaire)

Pour tout $\delta > 0$, $s \in [0,1]$, $s' \in \left[0, \frac{1}{2}\right]$, $\tau \geqslant \tau_0$, $u \in C_c^\infty(B_1 \setminus \{0\})$,

$$\tau^{3-4s} \left\|(-\Delta)^{(1-\delta)s}\left(e^{\tau\phi}u\right)\right\|_{L^2}^2 + \tau^{1-4s'} \sum_{i=1}^n \left\|(-\Delta)^{(1-\delta)s'}\left(e^{\tau\phi}\partial_i u\right)\right\|_{L^2}^2 \leqslant \frac{\kappa_n}{\delta^{5/2}} \left\|e^{\tau\phi}\Delta u\right\|_{L^2}^2 .$$

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- We use $|V_{\text{many-body}}|^2 \leqslant \epsilon(-\Delta)^{\frac{3}{2}-\delta} + c$

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Extensions

- **Interactions** :
  $\rho_\Psi^{(2)}(x,y) := \frac{N(N-1)}{2} \int_{\mathbb{R}^{d(N-2)}} |\Psi|^2 (x, y, x_3, \ldots, x_N) \mathrm{d}x_3 \cdots \mathrm{d}x_N$
  $\left\langle \Psi, \left(\sum_{1 \leqslant i < j \leqslant N} w(x_i - x_j) \right) \Psi \right\rangle = \int_{\mathbb{R}^{2d}} w(x-y) \rho_\Psi^{(2)}(x,y)$,
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- **Zeeman magnetism** : $H^N(v,B) := H^N(v) + \sum_{i=1}^N \sigma_i \cdot B(x_i),$
  $\left\langle \Psi, \left(\sum_{i=1}^N \sigma_i \cdot B(x_i)\right)\Psi\right\rangle = \int_{\mathbb{R}^d} B \cdot m_\Psi$
  $(v,B) \mapsto (\rho, m)$, "almost" injective

$$(\rho_{\Psi_1}, m_{\Psi_1}) = (\rho_{\Psi_2}, m_{\Psi_2}) \implies \boxed{|B_1 - B_2|\,\chi = \frac{E_1 - E_2}{N} + v_2 - v_1},$$

where $\chi(x) \in \{-1, -1+\frac{2}{N}, -1+\frac{4}{N}, \dots, 1-\frac{2}{N}, 1\}$

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- **At** $T > 0$**,** all HKs hold : $(T, v, A, w) \mapsto (S, \rho, j_{\mathrm{tot}}, \rho^{(2)})$ injective, non local $G \mapsto \gamma$, classical, (grand) canonical

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Plan

Definition of $v \mapsto \rho(v)$

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- $\Psi(v) :=$ ground state of $H^N(v)$,

$$\rho : \begin{array}{ccc} \mathcal{V}^N & \longrightarrow & W^{1,1}(\mathbb{R}^d, \mathbb{R}_+) \cap \{\int \cdot = N\} \\ v & \longmapsto & \rho_{\Psi(v)} = \rho(v), \end{array}$$

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- Is $\mathcal{V}^N$ path-connected ? Adiabatic equivalence ?

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Lemma

$\widetilde{\rho} : H^1_{\mathrm{p}} \to W^{1,1} \cap \{\int \cdot = N\}$ is $\mathcal{C}^\infty$

Regularity and compactness of $v \mapsto \rho(v)$

Theorem (Main properties of Ψ)

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- *Let $\Lambda \subset \mathbb{R}^d$ be a bounded open set. Assume $v \in \mathcal{V}^N$, $\boxed{v_n \rightharpoonup v}$ and $v_n \mathbb{1}_{\mathbb{R}^d \setminus \Lambda} \to v \mathbb{1}_{\mathbb{R}^d \setminus \Lambda}$. Then $E^N(v_n) \to E^N(v)$, $v_n \in \mathcal{V}^N$ for n large enough, and $\boxed{\Psi(v_n) \to \Psi(v)}$ in $H^1_{\rm p}$*

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  $\boxed{\mathrm{d}_v\Psi \text{ is compact}}$ *and not surjective*

- *Let $\Lambda \subset \mathbb{R}^d$ be a bounded open set. Assume $v \in \mathcal{V}^N$, $\boxed{v_n \rightharpoonup v}$ and $v_n \mathbb{1}_{\mathbb{R}^d\setminus\Lambda} \to v\mathbb{1}_{\mathbb{R}^d\setminus\Lambda}$. Then $E^N(v_n) \to E^N(v)$, $v_n \in \mathcal{V}^N$ for n large enough, and $\boxed{\Psi(v_n) \to \Psi(v)}$ in $H^1_{\rm p}$*

ρ and $\mathrm{d}_v\rho$ are injective when $p > \max(2d/3, 2)$

Corollaries: Hellman-Feynman

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Corollary (Hellmann-Feynman)

The energy E^N is $\mathcal{C}^\infty$ on $\mathcal{V}^N$, with

$$\left(\mathrm{d}_v E^N\right) u = \int_{\mathbb{R}^d} u\rho(v)$$

Corollaries : ill-posedness of the Kohn-Sham potential

Corollary (The set of v-representable densities is very small)

Consider that the system lives in a bounded open set $\Omega \subset \mathbb{R}^d$. Then $\boxed{v \mapsto \rho(v) \text{ is compact}}$, *$\rho^{-1}$ is discontinuous, and $\rho(\mathcal{V}^N)$ is a countable union of compact sets. Hence $\rho(\mathcal{V}^N)$ has empty interior in $W^{1,1} \cap \left\{ \int \cdot = N \right\}$.*

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For $v \in \rho^{-1}\left(\rho(\mathcal{V}^N) \cap \rho_{w=0}(\mathcal{V}^N_{w=0})\right)$, the Kohn-Sham potential

$$\boxed{v_{\text{ks}}(v) := \rho^{-1}_{w=0} \circ \rho(v)}$$

is ill-posed !

Inverse continuity

Proposition (Weak inverse continuity of Ψ)

Let $p > \max(2d/3, 2)$, $v, v_n \in \mathcal{V}^N$ such that $v_n - E^N(v_n)/N$ is bounded in $L^p + L^\infty$ and $\Psi(v_n) \to \Psi(v)$ in $H^2(\mathbb{R}^{dN})$. Then $v_n \to v$ a.e. up to a subsequence.

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Degenerate potentials

Proposition (Degenerate Hellman-Feynman)

The energy $v \mapsto E^N(v)$ is infinitely half Gateaux differentiable on the singular points $\mathcal{V}_\partial^N \backslash \mathcal{V}^N$, with

$$
{}^+\delta_v E^N(u) = \min \sigma\left(\mathcal{P}(v) u \mathcal{P}(v)\right) = \min_{\substack{\Psi \in \mathrm{Ker}\left(H^N(v) - E^N(v)\right) \\ \int |\Psi|^2 = 1}} \int \rho_\Psi u
$$

Similarly, ${}^-\delta_v E^N(u) = \max_{\Psi \ldots} \int \rho_\Psi u$. *If*
$\dim \mathrm{Ker}\left(H^N(v) - E^N(v)\right) = 2$ *with* Ψ_1, Ψ_2 *an orthonormal basis,*

$$
\begin{aligned}
{}^\pm\delta_v E^N(u) = &\frac{1}{2} \int u \left(\rho_{\Psi_1} + \rho_{\Psi_2}\right) \\
&\mp \frac{1}{2} \sqrt{\left(\int u \left(\rho_{\Psi_1} - \rho_{\Psi_2}\right)\right)^2 + 4 \left|\left\langle \Psi_1, \left(\textstyle\sum_i u_i\right) \Psi_2 \right\rangle\right|^2}.
\end{aligned}
$$

Degenerate potentials

Proposition

- *Let* $\dim \mathrm{Ker}\left(H^N(v) - E^N(v)\right) = 2$, *take* $\psi, \varphi \in \mathrm{Ker}\left(H^N(v) - E^N(v)\right)$ *with* $\psi \perp \varphi$. *The degeneracy is broken in no direction at first order if and only if* $\rho_\psi = \rho_\varphi$ *and* $\int_{\mathbb{R}^{d(N-1)}} \psi\varphi \mathrm{d}x_2 \cdots \mathrm{d}x_N = 0$

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- *Let* $v \in \mathcal{V}_\partial^N \backslash \mathcal{V}^N$ *be degenerate, and* $\boxed{w = 0}$. *Then* $\boxed{h \mapsto E^N(h) \text{ is not differentiable}}$ *at* v, *in particular* ${}^+\delta_v E^N(u) < {}^-\delta_v E^N(u)$ *for at least one direction* u

Plan

The v-representability problem

- Take a target density $\rho \geqslant 0$, $\int_{\mathbb{R}^d} \rho = N$. Does a v exists such that $\boxed{\rho_{\Psi(v)} = \rho}$, where $\Psi(v)$ is a ground state of $H^N(v)$?

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- Ideally we want exact, pure quantum states, $\mathbb{R}^d$, $T = 0$

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Regularization : relaxation

- $G_\rho(v) = E^N(v) - \int v\rho$ is not coercive in L^p ! Ex : $V \in L^1 \cap L^{p>1}$, $V \geqslant 0$, $V_n(x) := n^d V(nx)$, $\|V_n\|_{L^p}^p = n^{d(p-1)} \int V^p \to +\infty$ but $E^N(V_n) = 0$, and $\int V_n\rho \to \rho(0) \int V$ is bounded

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- Relax : $\rho_\Psi = \rho$ replaced by $\int \rho_\Psi \alpha_i = r_i \ (= \int \rho \alpha_i)$ for weigths $\alpha_i \in L^\infty(\Omega, \mathbb{R}_+)$, $i \in I$, $\sum_i \alpha_i = \mathbb{1}_\Omega$. For $r = (r_i)_i$, $r_i > 0$, $\sum_i r_i = N$,

$$F^{N,\boldsymbol{\alpha}}(r) := \inf_{\substack{\Psi \in H^1_a(\Omega^N) \\ \int \alpha_i \rho_\Psi = r_i \ \forall i \in I}} \left\langle \Psi, H^N(0)\, \Psi \right\rangle, \quad F^{N,\boldsymbol{\alpha}}_{\text{mix}}(r) := \inf_{\substack{\Gamma \in \mathcal{S}^N_{\text{mix}}(\Omega) \\ \int \alpha_i \rho_\Gamma = r_i \ \forall i \in I}} \mathrm{Tr}\, H^N(0)\Gamma$$

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- Dual : restriction to potentials $V = \sum_{i \in I} v_i \alpha_i$, $v = (v_i)_i \in \ell^\infty(I, \mathbb{R})$

$$G_{r,\boldsymbol{\alpha}}(v) := E^N\left(\sum_{i \in I} v_i \alpha_i\right) - \sum_{i \in I} v_i r_i,$$

Regularization : result

Theorem (Well-posedness of the dual problem)

Let I be finite. Then $\boxed{G_{r,\boldsymbol{\alpha}} \text{ is coercive}}$ *in $\ell^1(I,\mathbb{R})$, and there exists a unique maximizer. If moreover Ω is bounded, there is an N-particle ground mixed state Γ_v of $H^N\left(\sum_{i\in I} v_i\alpha_i\right)$ such that $\int \alpha_i \rho_{\Gamma_v} = r_i$ and*

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- We can represent ρ by taking $(r_\rho)_i := \int \rho\alpha_i$ and finer sequences of weights $\boldsymbol{\alpha}_n$
- For pure states, a similar theorem would hold for v-representability of densities, but with excited states, if we can prove a unique continuation like theorem

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Numerical inversion

- We consider a target density $\rho \geqslant 0$ with $\int \rho = N$ and the Hamiltonian without interaction

$$H^N_{w=0}(v) := \sum_{i=1}^{N} \big(-\Delta_i + v(x_i) \big).$$

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- Is $\rho\left(\mathcal{V}_\partial^N\right) = \left\{\rho_{\Psi(v)} \;\middle|\; v \in \mathcal{V}_\partial^N\right\}$ dense in $\left\{\rho \geqslant 0, \int \cdot = N\right\}$?

The gradient ascent algorithm

Maximize

$$G_\rho(v) := E^N(v) - \int_{\mathbb{R}^d} v\rho$$

Hellman-Feynman :

$$(\mathrm{d}_v G_\rho)\, u = \int_{\mathbb{R}^d} u\big(\rho(v) - \rho\big),$$

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- Convergence criterion :

$$\left\|\rho(v_n) - \rho\right\|_{L^1} / N \leqslant 10^{-3}$$

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$d = 1$

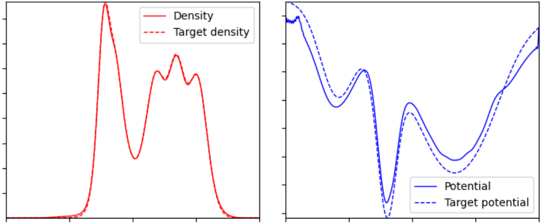

Figure: $d = 1$, $N = 5$, ground state (first line) and second excited state (second line)

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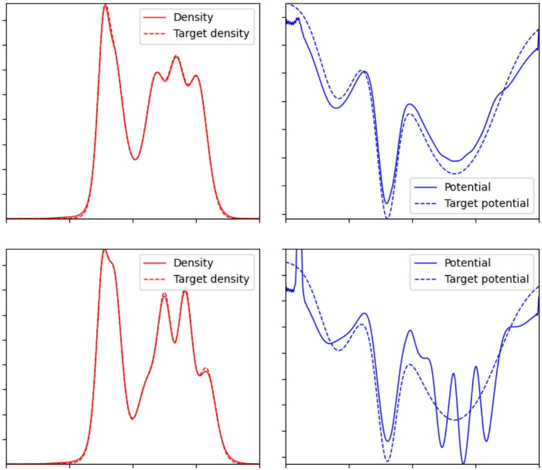

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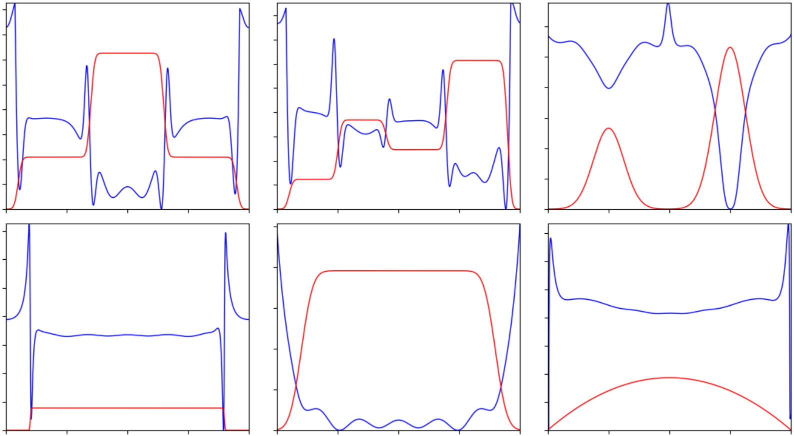

Figure: Target densities (red) and their Kohn-Sham potential (blue), for $d = 1$, $N = 5$

$d = 2$

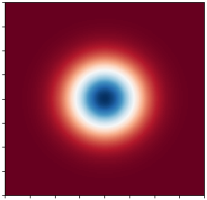

Figure: Gaussian target density, $N = 2$, the two ground state density configurations of potentials maximizing G_ρ, plot of $\|\rho(v_n) - \rho\|_{L^1} / N$ against n

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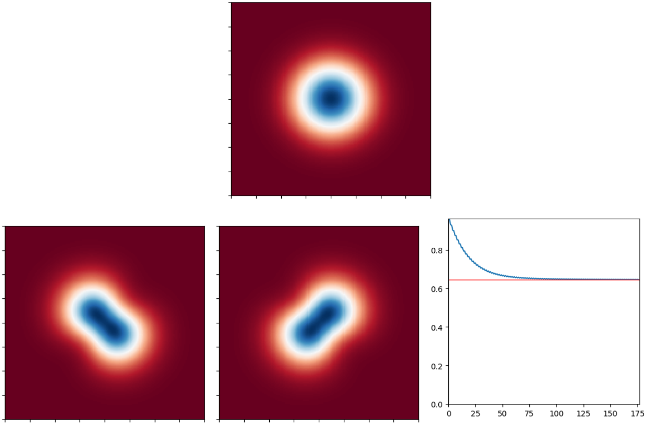

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For $d = 1$ and $N = 1$, for $v \in (L^1 + L^\infty)(\mathbb{R})$, every eigenstate of $H^N(v)$ is non-degenerate.

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- Close relationship between the Kohn-Sham potential, Levy and Levy-Lieb functionals, and degeneracy

$d = 2$, symmetry breaking

Take a familly

$$\rho_\alpha(x) := c_\alpha \left(e^{-\|x-x_0\|_2^2/(2\sigma^2)} + \alpha e^{-\|x+x_0\|_2^2/(2\sigma^2)} \right),$$

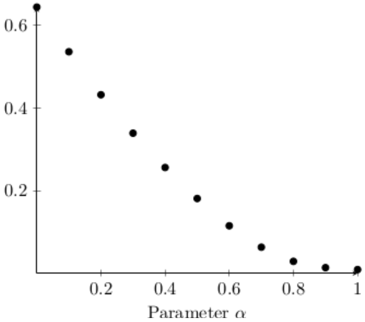

Figure: Plot of $\inf_{n\in\mathbb{N}} \|\rho(v_n) - \rho_\alpha\|_{L^1} / N$ against α, $N = 2$, $\sigma = 1$, $x_0 = (\sigma/5, 0)^T$

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- If the ground eigenspace of $H^N(v_{\mathrm{m}})$ is non-degenerate, then $v_{\mathrm{ks}} = v_{\mathrm{m}}$
- Otherwise, test if $\rho_\Psi = \rho$ for Ψ visiting $\mathrm{Ker}\left(H^N(v_{\mathrm{m}}) - E^N(v_{\mathrm{m}})\right)$

Improvements

- Use something better than gradient ascent, for fast convergence
- Adapt the code to get the mixed Kohn-Sham potential v_{m}
- If the Kohn-Sham potential v_{ks} exists, it is also the mixed Kohn-Sham v_{m}
- If the ground eigenspace of $H^N(v_{\mathrm{m}})$ is non-degenerate, then $v_{\mathrm{ks}} = v_{\mathrm{m}}$
- Otherwise, test if $\rho_\Psi = \rho$ for Ψ visiting $\mathrm{Ker}\left(H^N(v_{\mathrm{m}}) - E^N(v_{\mathrm{m}})\right)$
- If no, then the Kohn-Sham potential of ρ does not exist