Inverse potentials of one-body densities

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N-body quantum mechanics

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- Hamiltonian : operator of $L^2_a\left(\left(\mathbb{R}^d\right)^N, \mathbb{C}\right)$

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

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- Ground and excited states are given by the k^{th} eigenspaces $\text{Ker}\left(H_N(v) - E_N^{(k)}(v)\right)$, found by

$$E_N^{(k)}(v) = \sup_{\substack{A \subset L^2_a((\mathbb{R}^d)^N) \\ \dim_{\mathbb{C}} A = k}} \inf_{\substack{\Psi \in A^\perp \\ \int |\Psi|^2 = 1 \\ \Psi \in H^1_a((\mathbb{R}^d)^N)}} \langle \Psi, H_N(v)\Psi \rangle$$

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- Curse of dimensionality

Spectrum

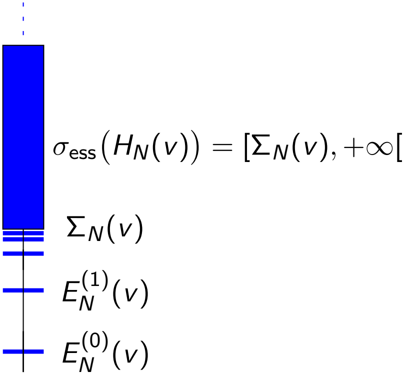

Figure: Spectrum $\sigma\left(H_N(v)\right)$

A k^{th} bound state exists if v is in

$$\mathcal{V}_{N,\partial}^{(k)} := \left\{ v \in L^p + L^\infty \;\middle|\; E_N^{(k)}(v) < \inf \sigma_{\text{ess}}(H_N(v)) \right\}$$

Pure and mixed states

- Pure states are

$$\left\{ P_\Psi = |\Psi\rangle \langle\Psi| \,, \Psi \in H^1_a(\mathbb{R}^{dN}), \int_{\mathbb{R}^{dN}} |\Psi|^2 = 1 \right\}$$

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- Choose a basis $(\Psi_i)_i$. Mixed states are

$$\begin{aligned}
\text{Conv } & \left\{ P_\Psi = |\Psi\rangle\langle\Psi|, \Psi \in H^1_{\mathrm{a}}(\mathbb{R}^{dN}), \int_{\mathbb{R}^{dN}} |\Psi|^2 = 1 \right\} \\
&= \left\{ \sum_{i \in \mathbb{N}} \lambda_i P_{\Psi_i} \mid \sum_{i=1}^{+\infty} \lambda_i = 1, \lambda_i \geqslant 0 \right\} \\
&= \left\{ \Gamma \text{ op of } H^1_{\mathrm{a}}(\mathbb{R}^{dN}) \mid \Gamma = \Gamma^* \geqslant 0, \operatorname{Tr} \Gamma = 1 \right\}
\end{aligned}$$

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$$k^{\text{th}} \text{ bound mixed states : } \mathrm{Ran}\,\Gamma \subset \mathrm{Ker}\left(H_N(v) - E_N^{(k)}(v) \right)$$

The one-body density

- One-body density (much less information than Ψ)

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

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- $\rho \geqslant 0$, $\int \rho_\Psi = N$, $\sqrt{\rho} \in H^1$

Inverse potential

- Given $\rho \geqslant 0$, $\int \rho = N$, $k \in \mathbb{N}$, find v such that $\rho_{\Psi^{(k)}(v)} = \rho$.

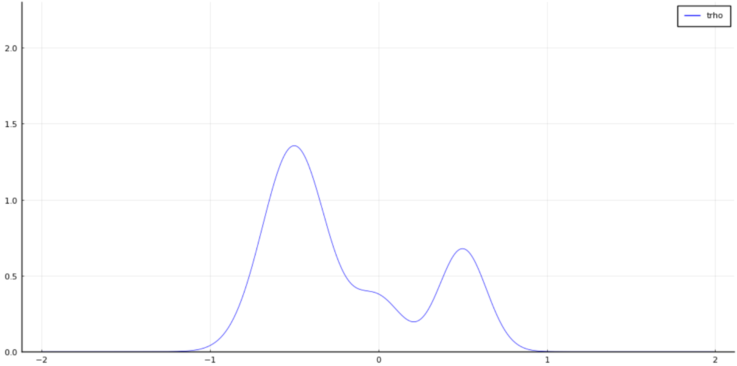

Figure: Density ρ for $N = 3$

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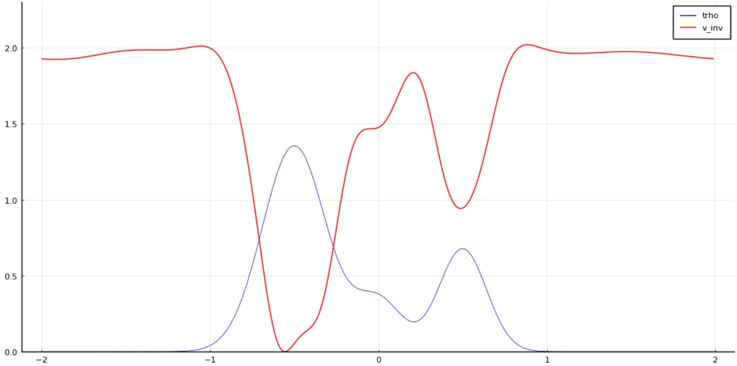

Figure: Density ρ and its inverse v, for $N = 3$ and $k = 2$

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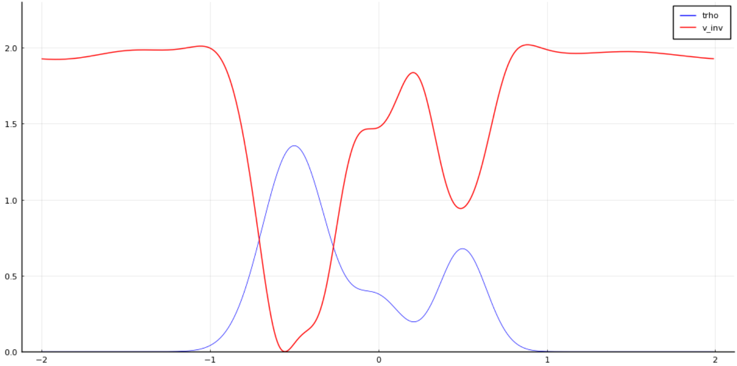

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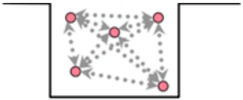
Existence/uniqueness ?

Why finding inverse potentials ?

- Finding effective models in DFT



$\longrightarrow$

$$\rho \longrightarrow H^N_{w=0}(v_{\text{eff}})$$

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$$\Psi^{(k)}, E_N^{(k)}, \ldots$$

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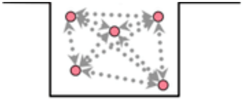

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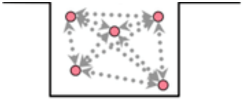

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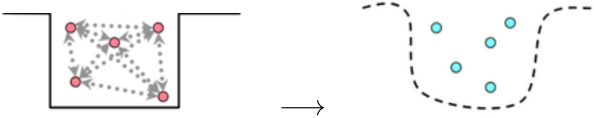

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- Control theory
- Mathematical understanding of DFT
- Optimal Effective Potential

Questions

$$\text{DFT map: } v \mapsto \rho_{\Psi^{(k)}(v)} = \rho^{(k)}(v)$$

Given $\rho \geqslant 0$, $\int \rho = N$, we search v_ρ such that

$$\boxed{\rho^{(k)}(v_\rho) = \rho}$$

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- Inverting algorithm ?

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The definition set

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Corollary (Path-connectedness of the set v-representable densities)

The set $\rho^{(0)}\left(\cap_{i=1}^N \mathcal{V}_{i,\partial}^{(0)}\right)$ *is path-connected*

Injectivity

Theorem (Hohenberg-Kohn, 1964)

Let $w, v_1, v_2 \in L^{p>\max(2,2d/3)}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$. *If there are two ground states* Ψ_1 *and* Ψ_2 *of* $H_N(v_1)$ *and* $H_N(v_2)$, *such that*

$$\rho_{\Psi_1} = \rho_{\Psi_2},$$

then $v_1 = v_2 + \frac{E_1 - E_2}{N}$.

Compactness of $v \mapsto \rho^{(0)}(v)$

Theorem (Main properties of $\Psi^{(0)}$)

- $v \mapsto \Psi^{(k)}(v)$ *is* $\mathcal{C}^\infty$ *from* $\mathcal{V}_N^{(k)}$ *to* H^1_{p}

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- *For $v \in \mathcal{V}_N^{(k)}$, $\mathrm{d}_v\Psi^{(k)} : L^{d/2} + L^\infty \to H^1 \cap \left\{\Psi^{(k)}(v)\right\}^\perp$*

$$\left(\mathrm{d}_v\Psi^{(k)}\right) u = -\left(H_N(v) - E_N^{(k)}(v)\right)_\perp^{-1} \left(\Sigma_{i=1}^N u(x_i)\right) \Psi^{(k)}(v),$$

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- *Let $\Lambda \subset \mathbb{R}^d$ be a bounded open set. Assume $v \in \mathcal{V}_N^{(0)}$, $\boxed{v_n \rightharpoonup v}$ and $v_n \mathbb{1}_{\mathbb{R}^d\setminus\Lambda} \to v\mathbb{1}_{\mathbb{R}^d\setminus\Lambda}$ in $L^{p>\frac{d}{2}} + L^\infty$. Then $E_N^{(0)}(v_n) \to E_N^{(0)}(v)$, $v_n \in \mathcal{V}_N^{(0)}$ for n large enough, and $\boxed{\Psi^{(0)}(v_n) \to \Psi^{(0)}(v)}$ in H^1*

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Ill-posedness of the inversion

Theorem (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 $\boxed{L^{p>d/2} \ni v \mapsto \rho^{(0)}(v) \in W^{1,1} \text{ is compact}}$, $(\rho^{(0)})^{-1}$ *is discontinuous, and* $\rho^{(0)}(\mathcal{V}_N^{(0)})$ *has empty interior in* $W^{1,1} \cap \{\int \cdot = N\}$.

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The inverse problem is ill-posed !

Inverse continuity

Proposition (Weak inverse continuity of Ψ)

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

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Existing literature

Target ρ: we search v such that

- $\rho_{\Psi^{(k)}(v)} = \rho$ for pure states, $\Psi^{(k)}(v) \in \mathrm{Ker}\left(H_N(v) - E_N^{(k)}(v)\right)$
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- quantum systems on lattices for $k = 0$ for mixed states (Chayes Chayes Ruskai 1985)

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Dual optimality

$$G_\rho^{(k)}(v) := E_N^{(k)}(v) - \int_{\mathbb{R}^d} v\rho, \qquad \sup_{v \in L^p(\mathbb{R}^d)} G_\rho^{(0)}(v) = F_{\mathrm{L}}(\rho)$$

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- Concave for $k = 0$

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- $G_\rho^{(k)}(v+c) = G_\rho^{(k)}(v)$
- Concave for $k = 0$
- On degenerate potentials, $v \mapsto \rho_{\Psi^{(k)}(v)}$ and $E_N^{(k)}$ are not differentiable

Dual optimality

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Does a maximum exist ?

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Regularization

- $G_\rho^{(k)}(v) = E_N^{(k)}(v) - \int v\rho$ 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 $E_N^{(k)}(v_n) = 0$, and $\int v_n\rho \to \rho(0) \int v$ is bounded

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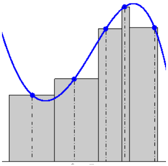
  $\int v_n\rho \to \rho(0) \int v$ is bounded
- Dual : restriction to potentials $V = \sum_{i\in I} v_i\alpha_i$,
  $v \in (v_i)_{i\in I} \in \ell^\infty(I,\mathbb{R})$, $\alpha_i \in L^\infty(\Omega)$, $\sum_{i\in I}\alpha_i = \mathbb{1}_\Omega$, $r_i \in \mathbb{R}_+$,
  $r_i = \int \rho\alpha_i$, $\sum_{i\in I} r_i = N$

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



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$$G_{r,\alpha}^{(k)}(v) \leqslant -\frac{\min r}{N} \|v\|_{\ell^1} + c,$$

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When I is finite $G^{(k)}_{r,\boldsymbol{\alpha}}$ is coercive and there exists a maximizer v. If $\Omega \subset \mathbb{R}^d$ is bounded, there is a k^{th} excited N-particle ground mixed state Γ_v of $H_N\left(\sum_{i\in I} v_i \alpha_i\right)$ such that $\int \alpha_i \rho_{\Gamma_v} = r_i$ $(= \int \alpha_i \rho)$ $\forall i$.

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- **Constructive inversion with mixed states**
  For a given k, ρ, $\varepsilon > 0$, there exists a potential v and Γ_v with $\operatorname{Ran}\Gamma_v \subset \operatorname{Ker}\left(H_N(v) - E_N^{(k)}(v)\right)$ such that $\|\rho_{\Gamma_v} - \rho\|_{L^1\cap L^q} \leqslant \varepsilon$. The state can be chosen to be **pure** when $d = 1$ and $w = 0$.

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"Gradient" ascent

Minimize $J(v) := \int_{\mathbb{R}^d} \left(\rho_{\Psi^{(k)}(v)} - \rho \right)^2$?

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Second idea, maximize

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Local dual problem

$$
{}^{+}\delta_v G_\rho^{(k)}(u) = \max_{\substack{\Psi_0,\dots,\Psi_{M_k-k}\in \mathrm{Ker}\left(H_N(v)-E_N^{(k)}(v)\right) \\ \|\Psi_i\|=1,\Psi_i\perp\Psi_j \\ 0\leqslant i,j\leqslant M_k-k}} \; \min_{\substack{\Psi=\sum_{i=0}^{M_k-k}\lambda_i\Psi_i \\ \lambda_i\in\mathbb{C},\sum_i|\lambda_i|^2=1}} \int (\rho_\Psi - \rho)\, u
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Proposition (Local dual problem)

Take $w \geqslant 0$, $v \in \mathcal{V}_{N,\partial}^{(k)}$. We have

$$ \sup_{\substack{u\in L^p+L^\infty \\ \|u\|_{L^p+L^\infty}=1}} {}^{+}\delta_v G_\rho^{(k)}(u) = \max_{\substack{Q\subset \mathrm{Ker}_{\mathbb{R}}(H_N(v)-E_N^{(k)}(v)) \\ \dim_{\mathbb{R}} Q = M_k-k+1}} \min_{\substack{\Gamma\in\mathcal{S}(Q) \\ \Gamma\geqslant 0, \mathrm{Tr}\,\Gamma=1}} \|\rho_\Gamma-\rho\|_{L^{p'}}, $$

and the supremum is attained by $u^* = \left|\frac{\rho_{\Gamma^*}-\rho}{\|\rho_{\Gamma^*}-\rho\|_{L^{p'}}}\right|^{p'-1} \mathrm{sgn}(\rho_{\Gamma^*}-\rho)$, *where Γ^* is an optimizer of the right hand side.*

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- Convergence criterion: $\left\|\rho^{(k)}(v_n) - \rho\right\|_{L^1} / N \leqslant \varepsilon$

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- Approximate inversion with mixed states for any k

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What we want to know

- Uniqueness for $k \geqslant 1$?
- Inversion with pure states for $d = 2$?

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$d = 1$

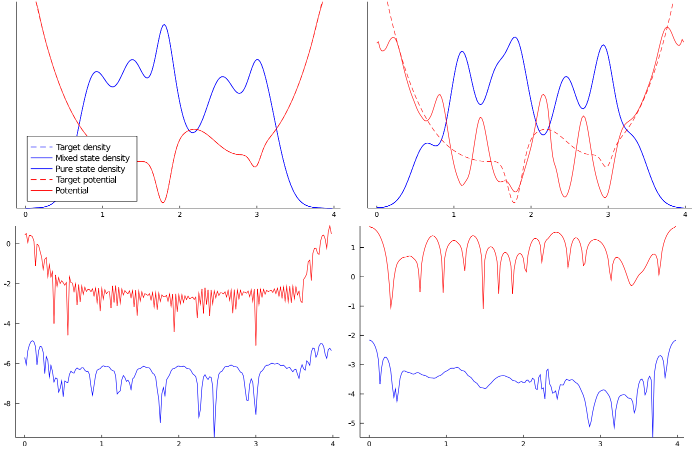

Figure: Plot for $d = 1$, $N = 5$, $k = 0$ on the left, $k = 3$ on the right, $\log_{10}|\rho_n - \rho|$, $\log_{10}|v_n - v|$

Uniqueness

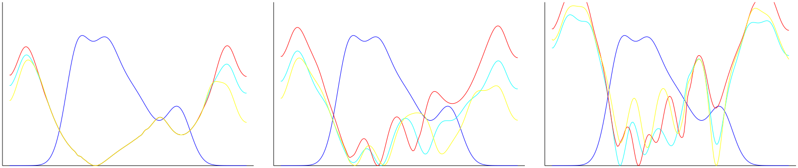

Figure: $d = 1$, $N = 3$, $k = 0$ left, $k = 1$ middle, $k = 5$ right. Densities in blue, inverse potentials in other colors

$d = 2$

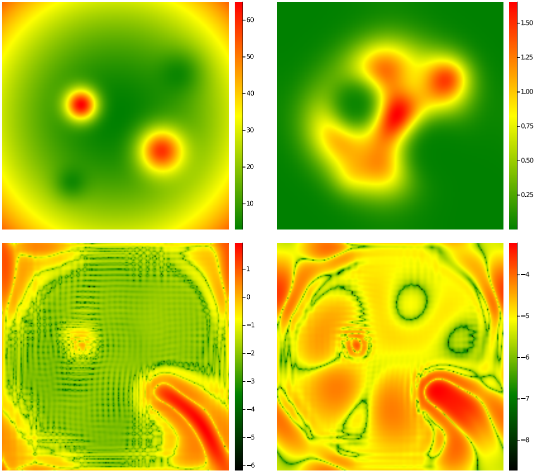

Figure: $d = 2,\ N = 5,\ k = 0\ ;\ v,\ \rho_{\Psi^{(0)}(v)},\ \log_{10}|v_n - v|,$
$\log_{10}\left|\rho_n - \rho_{\Psi^{(0)}(v)}\right|$

$d = 3$

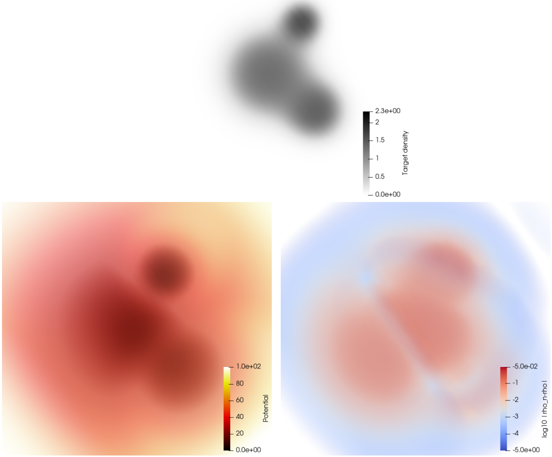

Figure: $d = 3,\ N = 4,\ k = 1\ ;\ \rho,\ v_n,\ \log_{10} |\rho_n - \rho|$

Simulations at high densities

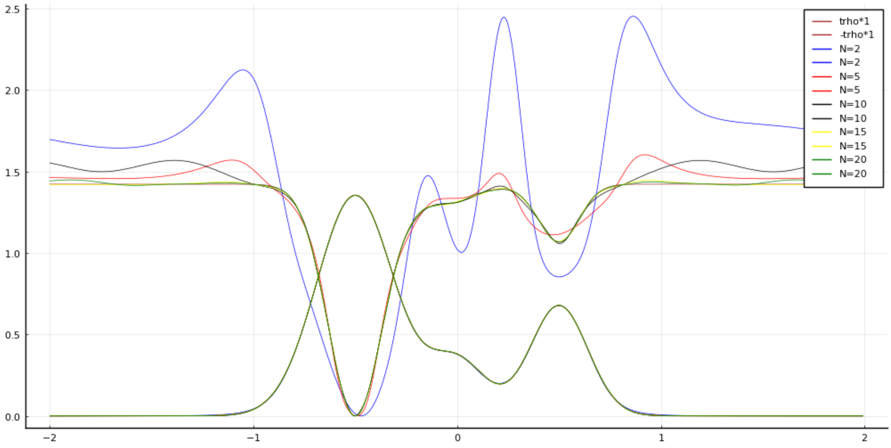

Figure: Convergence of $\rho_N^{-1}(N\rho)/N^{\frac{2}{d}}$, $\int \rho = 1$

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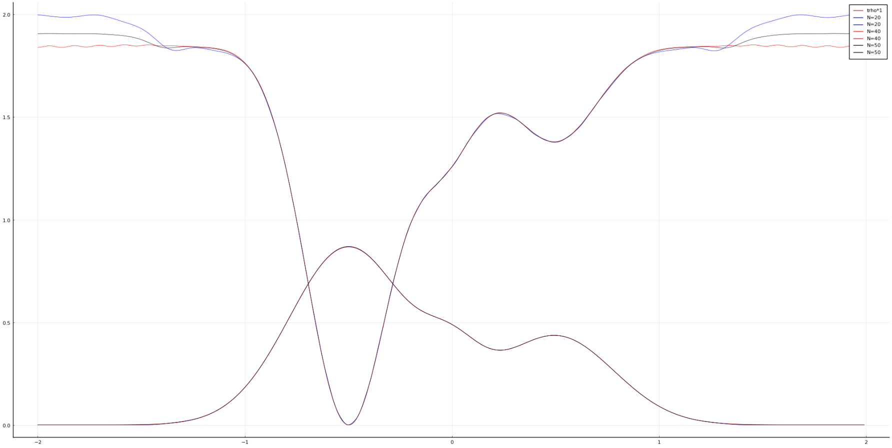

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Conjecture

For any $\rho \geqslant 0$ such that $\int \rho = 1$ and $\sqrt{\rho} \in H^1$,

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The direct statement version is in Founais, Lewin, Solovej (2019)

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What we learn from simulations

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- Degeneracies are generic, even for $d = 1$. Need to be considered, not in literature

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- We gave an algorithm taking into account degeneracies