Inverse potentials of one-body densities

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Table of contents

Table of contents

Table of contents

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 states are given by the eigenspace $\mathrm{Ker}\left(H_N(v) - E_N(v)\right)$, found by

$$E_N(v) = \inf_{\substack{\Psi \in H^1_a((\mathbb{R}^d)^N) \\ \int |\Psi|^2 = 1}} \langle \Psi, H_N(v)\Psi \rangle$$

Pure and mixed states

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- Choose a basis $(\Psi_i)_{i\in\mathbb{N}}$. Mixed states are

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

ground mixed states : $\mathrm{Ran}\,\Gamma \subset \mathrm{Ker}\,(H_N(v) - E_N(v))$

The one-body density

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

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

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

Table of contents

Inverse potential

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

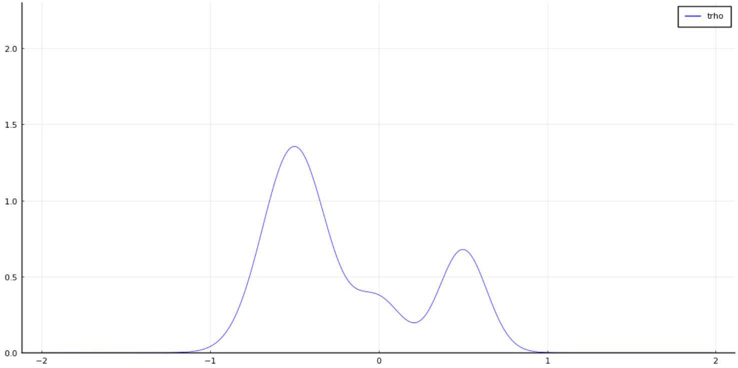

Figure: Density ρ and its inverse v, for $N = 3$ and $k = 2$

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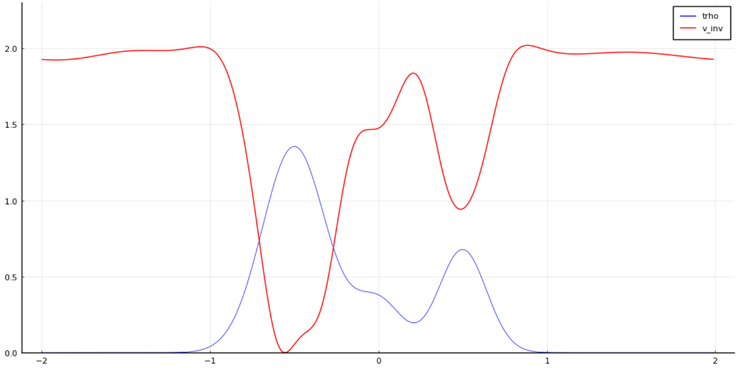

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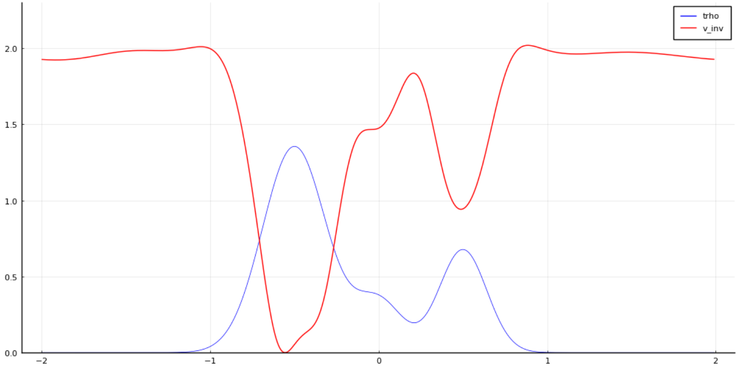

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Existence/uniqueness ?

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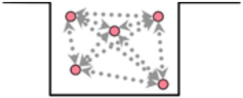

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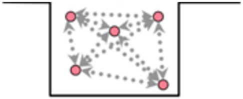

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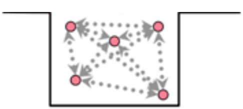 $\longrightarrow$ 

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$$\downarrow$$

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

Questions

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

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

$$\boxed{\rho^{\mathrm{HK}}(v_\rho) = \rho}$$

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- Is the inverse problem well-posed ?
- How to invert it algorithmically ?

Table of contents

Table of contents

ρ contains everything

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

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- Implies existence of functionals for any quantity
- Lieb (1964) remarked it relies on SUCP. Conjectures $L^{\frac{3}{2}}(\mathbb{R}^3)$, other mathematicians interested

Strong UCP

Theorem (Strong UCP for many-body Schrödinger operators)

Assume that the potentials satisfy $v, w \in L^p_{\mathrm{loc}}(\mathbb{R}^d)$ *with* $p > \max\left(\frac{2d}{3}, 2\right)$. *If* $\Psi \in H^2_{\mathrm{loc}}(\mathbb{R}^{dN})$ *is a non zero solution to* $H_N(v)\Psi = E\Psi$, *then* $|\{\Psi(X) = 0\}| = 0$.

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- Lammert (2018) ; Laestadius, Benedicks, Penz (2020)
- This L^p result uses technics developped by Carleman, Hörmander, Koch and Tataru

Table of contents

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

Theorem (Main properties of Ψ)

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

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- *$v \mapsto \Psi(v)$ is $\mathcal{C}^\infty$ from $\mathcal{V}_N$ to H^1_{p}*
- *For $v \in \mathcal{V}_N$, $\mathrm{d}_v\Psi : L^{d/2} + L^\infty \to H^1 \cap \{\Psi(v)\}^\perp$*

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

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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 $v_n \mathbb{1}_{\mathbb{R}^d\setminus\Lambda} \to v\mathbb{1}_{\mathbb{R}^d\setminus\Lambda}$ in $L^{p+\epsilon} + L^\infty$. 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*

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 $\boxed{L^{p>d/2} \ni v \mapsto \rho^{HK}(v) \in W^{1,1} \text{ is weak-strong continuous}}$, *$(\rho^{HK})^{-1}$ is discontinuous, and $\rho^{HK}(L^p(\mathbb{R}^d))$ has empty interior in $W^{1,1} \cap \{\int \cdot = N\}$.*

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Table of contents

Table of contents

Existing literature

Target ρ: we search v such that

- $\rho_{\Psi(v)} = \rho$ for pure states, $\Psi(v) \in \mathrm{Ker}\,(H_N(v) - E_N(v))$
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- Numerical articles

Table of contents

Dual optimality

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

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i) The following statements are equivalent

- *there is a* k^{th} *bound mixed state* Γ *of* v *such that* $\rho_\Gamma = \rho$
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ii) If v *maximizes* $G_\rho^{(k)}$ *and*

- $\dim \operatorname{Ker}\left(H_N(v) - E_N(v)\right) \in \{1, 2\}$,
- *or* $d = 1$ *and* $w = 0$,

then v *has a* k^{th} *bound pure state* Ψ *such that* $\rho_\Psi = \rho$.

Dual optimality

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

Theorem (Optimality in the dual problem)

Take $w \geqslant 0$, $\rho \in L^1(\mathbb{R}^d)$, $\rho \geqslant 0$, $\int \rho = N$, $\sqrt{\rho} \in H^1(\mathbb{R}^d)$, $v \in L^{p>2}$ *such that* $H_N(v)$ *has a ground state.*

i) The following statements are equivalent

- *there is a* k^{th} *bound mixed state* Γ *of* v *such that* $\rho_\Gamma = \rho$
- v *is a local maximizer of* $G_\rho^{(k)}$
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ii) If v *maximizes* $G_\rho^{(k)}$ *and*

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Does a maximum exist ?

Table of contents

Regularization

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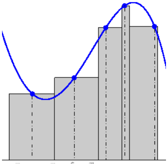
- Dual : restriction to potentials $V = \sum_{i \in I} v_i \alpha_i$,
  $v \in (v_i)_{i \in I} \in \ell^\infty(I, \mathbb{R})$, $\alpha_i \in L^\infty(\Omega)$, $\sum_{i \in I} \alpha_i = \mathbb{1}_\Omega$, $r_i \in \mathbb{R}_+$,
  $r_i = \int \rho \alpha_i$, $\sum_{i \in I} r_i = N$

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



Coercivity

$$G_{r,\alpha}^{(k)}(v) \leqslant -\min\left(1, \frac{\sum_{v_i \geqslant c_\Omega} r_i}{\sum_{v_i < c_\Omega} r_i}\right) \|v - c_\Omega\|_{\ell_r^1} + c_R,$$

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Theorem (Existence of the inverse potential)

When I is finite $G_{r,\alpha}^{(k)}$ 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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- $\boxed{\text{Constructive inversion with mixed states}}$

  For a given ρ, $\epsilon > 0$, there exists a potential v and Γ_v with $\operatorname{Ran} \Gamma_v \subset \operatorname{Ker}\left(H_N(v) - E_N(v)\right)$ such that $\|\rho_{\Gamma_v} - \rho\|_{L^1 \cap L^q} \leqslant \epsilon$.

Table of contents

Table of contents

"Gradient" ascent

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

"Gradient" ascent

Minimize $J(v) := \int_{\mathbb{R}^d} \left(\rho_{\Psi(v)} - \rho\right)^2$?
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(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 $w \geqslant 0$, $v \in \mathcal{V}_{N,\partial}$. We have

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

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: $\left\|\rho^{\mathrm{HK}}(v_n) - \rho\right\|_{L^1} / N \leqslant \epsilon$

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What we know

- Approximate inversion with mixed states for any k

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$$\Big\{\rho_{\Psi_v} \;\Big|\; v \in (L^p + L^\infty)(\Omega),\\ \Psi_v \in \mathrm{Ker}\left(H_N^{w=0}(v) - E_N(v)\right), \int_{\Omega^N} |\Psi_v|^2 = 1\Big\}$$

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What we want to know

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

Table of contents

$d = 1$

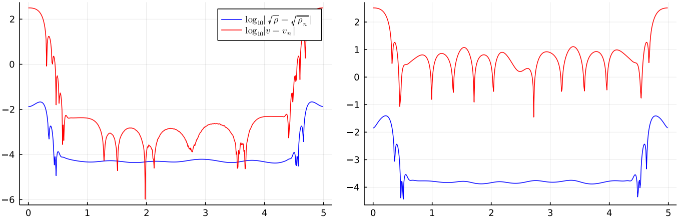

Figure: Plot for $d = 1$, $N = 5$, $k = 0$ on the left, $k = 3$ on the right, $\log_{10}|\rho_n - \rho|$, $\log_{10}|v_n - v|$

Uniqueness

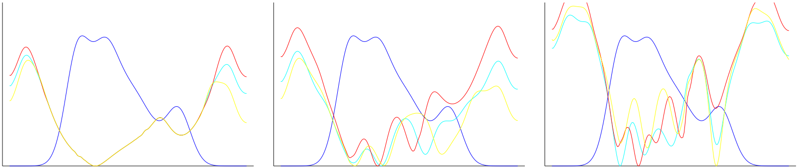

Figure: $d = 1$, $N = 3$, $k = 0$ left, $k = 1$ middle, $k = 5$ right. Densities in blue, inverse potentials in other colors

$d = 2$

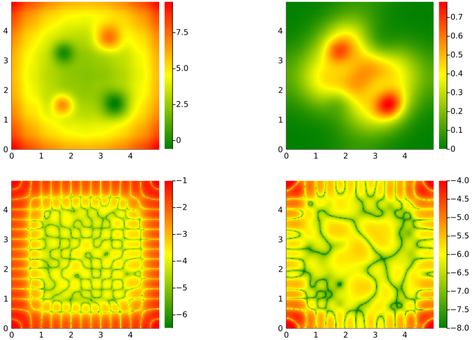

Figure: $d = 2$, $N = 5$, $k = 0$; v, $\rho_{\Psi^{(\mathbf{0})}(v)}$, $\log_{10}|v_n - v|$, $\log_{10}\left|\rho_n - \rho_{\Psi^{(\mathbf{0})}(v)}\right|$

$d = 3$

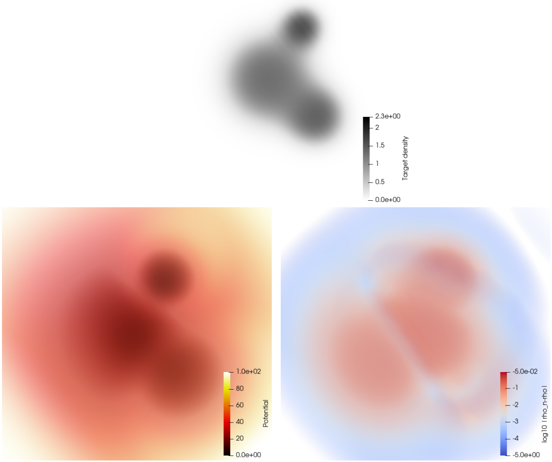

Figure: $d = 3,\ N = 4,\ k = 1$; $\rho,\ v_n,\ \log_{10}|\rho_n - \rho|$

Simulations at high densities

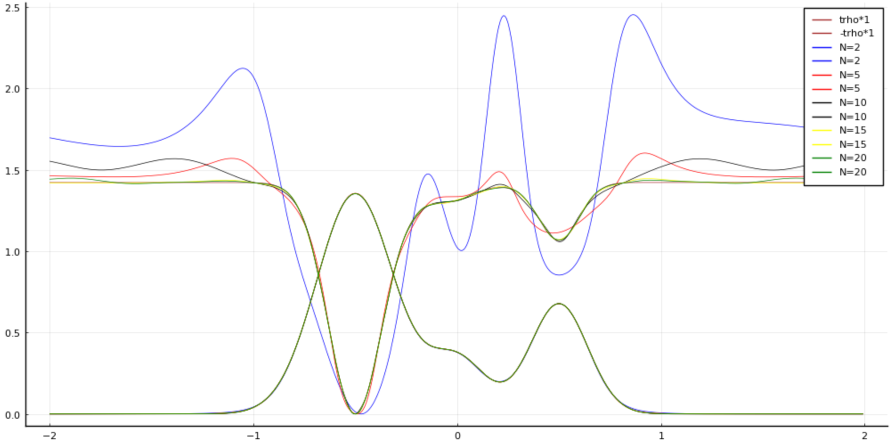

Figure: Convergence of $\rho_N^{-1}(N\rho)/N^{\frac{2}{d}}$, $\int \rho = 1$

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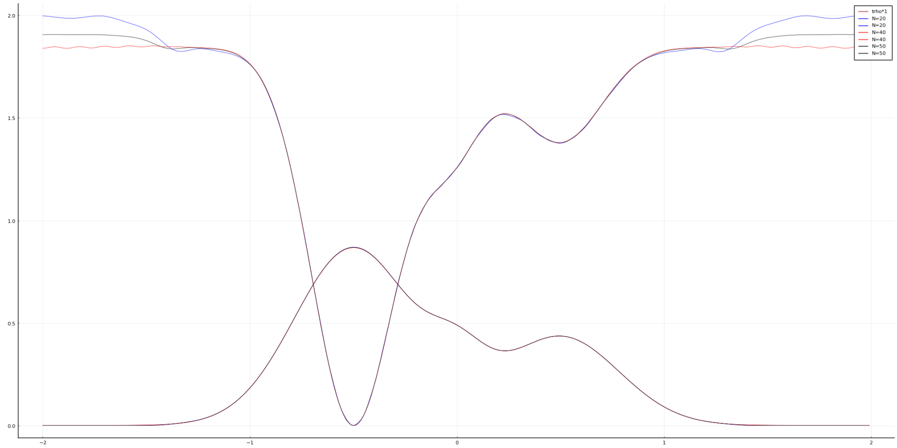

Figure: Convergence of $\rho_N^{-1}(N\rho)/N^{\frac{2}{d}}$, $\int \rho = 1$

Conjecture

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

$$\frac{\rho_N^{-1}(N\rho)}{N^{\frac{2}{d}}} \underset{N \to +\infty}{\longrightarrow}$$

Conjecture

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

$$\frac{\rho_N^{-1}(N\rho)}{N^{\frac{2}{d}}} \underset{N \to +\infty}{\longrightarrow} v_{\mathrm{TF},\rho} = -\rho^{\frac{2}{d}}$$

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

Table of contents

Statement

Theorem

Take $w \in (L^p + L^\infty)(\mathbb{R}^d, \mathbb{R}_+)$. Let $\boldsymbol{\alpha}$ be a partition of unity of Ω, with $\alpha_i \in L^\infty(\Omega, \mathbb{R}_+)$, such that we have $R > 0$ for which

$$(\operatorname{supp} \alpha_i) \setminus \cup_{j \in I, j \neq i} \operatorname{supp} \alpha_j$$

contains a ball of radius R, uniformly in $i \in I$. Let $r \in \ell^1(I, \mathbb{R}_+)$ be such that $\sum_{i \in I} r_i = N$ and $r_i > 0$ for all $i \in I$. For any $v \in \ell^1_r(I, \mathbb{R})$ such that $E_N\left(\sum_{i \in I} v_i \alpha_i\right) = 0$, we have

$$\boxed{G^{(k)}_{r,\boldsymbol{\alpha}}(v) \leqslant -\min\left(1, \frac{\sum_{v_i \geqslant c_\Omega} r_i}{\sum_{v_i < c_\Omega} r_i}\right) \|v - c_\Omega\|_{\ell^1_r} + c_R}$$

Proof

- We assumed that there are points $y_i \in \mathbb{R}^d$ such that for any $i \in I$,

$$B_R(y_i) \subset (\operatorname{supp} \alpha_i) \setminus \cup_{j \in I, j \neq i} \operatorname{supp} \alpha_j.$$

We write $X = (x_1, \ldots, x_N)$ and $Y_i := (y_i, \ldots, y_i)$. Take normalized $\Phi_0, \ldots, \Phi_k \in \wedge^N H_0^1(B_R)$ with disjoint supports. Take some non-empty $Q \subset I$ and for $j \in \{0, \ldots, k\}$, form

$$\Psi_{j,Q}(X) := \frac{1}{\sqrt{\sum_{i \in Q} r_i}} \sum_{i \in Q} \sqrt{r_i}\ \Phi_j(X - Y_i).$$

This satisfies $\int_{\Omega^N} |\Psi_{j,Q}|^2 = 1$, $T(\Psi_{j,Q}) = T(\Phi_j)$, $W(\Psi_{j,Q}) = W(\Phi_j)$ and

$$\rho_{\Psi_{j,Q}}(x) = \left(\sum_{i\in Q} r_i\right)^{-1} \sum_{i\in Q} r_i \rho_{\Phi_j}(x - y_i).$$

We use the expression

$$E_N^{(k)}(V) = \inf_{\dim A = k+1} \max_{\substack{\Psi\in A \\ \int_{\Omega^N}|\Psi|^2=1}} \mathcal{E}_V(\Psi)$$

and choose the frame $A := \left(\Psi_{0,Q}, \dots, \Psi_{k,Q}\right)$ so that

$$G_{r,\alpha}^{(k)}(v) \leqslant -\sum_{i\in I} v_i r_i + \max_{\substack{\lambda_j\in\mathbb{C} \\ \sum_{j=0}^k |\lambda_j|^2=1}} \mathcal{E}_{V(v)}\left(\sum_{j=0}^k \lambda_j \Psi_{j,Q}\right).$$

For any $i \in I$, the only non-vanishing element of $\boldsymbol{\alpha}$ in $B_R(y_i)$ is α_i, so $\alpha_i = 1$ on $B_R(y_i)$ and

$$\int_\Omega \alpha_i \rho_{\Psi_{j,Q}} = \frac{N r_i \delta_{i\in Q}}{\sum_{\ell\in Q} r_\ell},$$

$$\int_\Omega V(v)\rho_{\sum_{j=0}^k \lambda_j \Psi_{j,Q}} = \sum_{j=0}^k |\lambda_j|^2 \int_\Omega V(v)\rho_{\Psi_{j,Q}} = \frac{N\sum_{i\in Q} v_i r_i}{\sum_{\ell\in Q} r_\ell}.$$

We see that the external potential energy of the trial state does not depend on the λ_j's. Defining $c_R := \max_{\substack{\lambda_j\in\mathbb{C} \\ \sum_{j=0}^k |\lambda_j|^2=1}} \mathcal{E}_0\left(\sum_{j=0}^k \lambda_j \Psi_{j,Q}\right)$,

we deduce that

$$\begin{aligned} G_{r,\boldsymbol{\alpha}}(v) &\leqslant c_R + \frac{N}{\sum_{i\in Q} r_i}\sum_{i\in Q} v_i r_i - \sum_{i\in I} v_i r_i \\ &= c_R + \frac{\sum_{i\in I\setminus Q} r_i}{\sum_{i\in Q} r_i}\sum_{i\in Q} v_i r_i - \sum_{i\in I\setminus Q} v_i r_i. \end{aligned}$$

Since G is gauge invariant, for any $\mu \in \mathbb{R}$ and any non-empty $Q \subset I$, we have

$$G_{r,\alpha}(v) = G_{r,\alpha}(v-\mu) \leqslant c_R + \frac{\sum_{I\setminus Q} r_i}{\sum_{i\in Q} r_i} \sum_{i\in Q}(v_i-\mu)r_i - \sum_{i\in I\setminus Q}(v_i-\mu)r_i.$$

We define the two sets $I_v^{\pm} := \left\{ i \in I \;\middle|\; \pm v_i > \pm c_\Omega \right\}$. In the case $I_v^- \neq \varnothing$, we take $Q = I_v^-$ and $\mu = c_\Omega$ yielding

$$\begin{aligned}
G_{r,\alpha}(v) - c_R &\leqslant \frac{\sum_{v_i \geqslant c_\Omega} r_i}{\sum_{v_i < c_\Omega} r_i} \sum_{v_i < c_\Omega}(v_i - c_\Omega)r_i - \sum_{v_i \geqslant c_\Omega}(v_i - c_\Omega)r_i \\
&\leqslant \min\left(1, \frac{\sum_{v_i \geqslant c_\Omega} r_i}{\sum_{v_i < c_\Omega} r_i}\right)\left(\sum_{v_i < c_\Omega}(v_i - c_\Omega)r_i - \sum_{v_i \geqslant c_\Omega}(v_i - c_\Omega)r_i\right) \\
&\leqslant -\frac{\sum_{v_i \geqslant c_\Omega} r_i}{N} \left\| v - c_\Omega \right\|_{\ell_r^1}.
\end{aligned}$$

Table of contents

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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  - $d = 2$ yes (simulations)
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