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Computer-assisted existence proofs for one-dimensional Schrödinger-Poisson systems

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Outline

- Schrödinger-Poisson systems
- Theory of computer-assisted proofs
  - Setting
  - Existence and enclosure theorem
- Application to the one-dimensional Schrödinger-Poisson system
  - Approximate solution $\tilde{u}$
  - Defect bound δ
  - Norm bound for L^{-1}
  - Non-decreasing function g
  - Results

The three-dimensional time-dependent Schrödinger-Poisson system

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Starting point:

$$\left.\begin{aligned} -i\hbar\partial_t\psi - \frac{\hbar^2}{2m}\Delta\psi + q_e W_e \psi &= f(\psi) \\ -\varepsilon \Delta W_e &= q_e|\psi|^2 \end{aligned}\right\} \text{ on } [0,\infty)\times\mathbb{R}^3,$$

$$\lim_{|x|\to\infty} W_e = 0$$

- wavefunction ψ,
- mass m,
- electric potential W_e,
- elementary electric charge q_e,
- Planck's constant $\hbar$,
- nonlinearity f.

The one-dimensional Schrödinger-Poisson system

Goal:
Non-trivial solutions of the one-dimensional stationary Schrödinger-Poisson system

$$\left.\begin{aligned} -u'' + Vu + \Phi_u u &= f(u) \\ -\Phi_u'' + c\Phi_u &= u^2 \end{aligned}\right\} \text{ on } \mathbb{R},$$
$$\lim_{x \to \pm\infty} \Phi_u = 0$$

where $c > 0$, $V \in \mathrm{L}^\infty(\mathbb{R})$ is a positve potential and $f \in \mathrm{C}^1(\mathbb{R})$.

Additional property of the potential:

$$V^\infty := \lim_{x \to \pm\infty} V(x) > 0.$$

The one-dimensional Schrödinger-Poisson system

Using the Green's function Γ for $-\Phi'' + c\Phi$:

$$\Phi_u = \int_{\mathbb{R}} \Gamma(\cdot, t) u(t)^2 \, dt.$$

Insert into the first equation:

$$-u'' + \left(V + \int_{\mathbb{R}} \Gamma(\cdot, t) u(t)^2 \, dt\right) u = f(u) \text{ on } \mathbb{R}, \tag{SPS}$$

where $u \in \mathrm{H}^1(\mathbb{R})$.

Spaces

Inner product on $H^1(\mathbb{R})$:

$$\langle u, v\rangle_{H^1} := \langle u', v'\rangle_{L^2} + \sigma \langle u, v\rangle_{L^2} \quad (u, v \in H^1(\mathbb{R})).$$

with $\sigma > 0$ to be chosen later.

Spaces:

- $H^1_S(\mathbb{R}) := \{u \in H^1(\mathbb{R}) \colon u(x) = u(-x) \ (x \in \mathbb{R})\}$
- $H^{-1}_S(\mathbb{R}) := \left(H^1_S(\mathbb{R})\right)'$

Canonical isometric isomorphism:

$$\Phi\colon \ H^1_S(\mathbb{R}) \to H^{-1}_S(\mathbb{R}), \ u \mapsto \langle u, \cdot\rangle_{H^1}$$

Setting

Define $F\colon\ \mathrm{H}^1_S(\mathbb{R}) \to \mathrm{H}^{-1}_S(\mathbb{R})$ by

$$(Fu)[v] := \int_{\mathbb{R}} \left[u'v' + \left(V + \int_{\mathbb{R}} \Gamma(\cdot, t) u(t)^2 \, dt \right) uv - f(u)v \right] dx.$$

Let some approximate solution $\tilde{u} \in \mathrm{H}^1_S(\mathbb{R})$ of $Fu = 0$ be computed (A0)

Linearization of F at $\tilde{u}$:

$$L\colon\ \mathrm{H}^1_S(\mathbb{R}) \to \mathrm{H}^{-1}_S(\mathbb{R}),\ L = F'\tilde{u}$$

Nonlinearity: $f(y) = y^3$ $(y \in \mathbb{R})$.

Constant potential: $V \equiv V_0 > 0$.

Assumptions

Need constants $\delta \geq 0$, $K \geq 0$ and a non-decreasing function $g\colon [0,\infty) \to [0,\infty)$ satisfying:

- Bound for the defect (residual) of $\tilde{u}$:

$$\|F\tilde{u}\|_{H^{-1}} \leq \delta, \tag{A1}$$

- Norm bound for L^{-1}:

$$\|u\|_{H^1} \leq K\,\|Lu\|_{H^{-1}} \quad \left(u \in H^1_S(\mathbb{R})\right), \tag{A2}$$

- $\left\|F'(\tilde{u}+u) - F'\tilde{u}\right\|_{\mathcal{B}} \leq g(\|u\|_{H^1}) \quad \left(u \in H^1_S(\mathbb{R})\right),$ (A3)
- $g(t) \to 0 \ (t \to 0^+).$ (A4)

Existence and enclosure theorem

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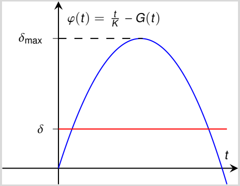
Theorem (Existence and enclosure theorem, see [4])

Let $\tilde{u} \in H^1_S(\mathbb{R})$ *be an approximate solution of* $Fu = 0$*, i.e. of (SPS). Moreover let* $\tilde{u}, \delta, K$ *and* $g\colon [0,\infty) \to [0,\infty)$ *satisfy the assumptions (A1) - (A4).*

Suppose some $\alpha \geq 0$ *exists, such that*

$$\delta \leq \frac{\alpha}{K} - G(\alpha) \quad \text{and}$$
$$K \cdot g(\alpha) < 1,$$



where $G(s) = \int_0^s g(t)\,dt$.

Then there exists an exact solution $u^* \in H^1_S(\mathbb{R})$ *of* $Fu = 0$*, satisfying the enclosure*

$$\left\|u^* - \tilde{u}\right\|_{H^1} \leq \alpha.$$

(A0) Approximate solution $\tilde{u}$

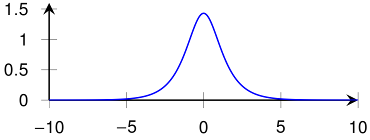
Look for approximations in $V^S_{R,M} = \operatorname{span}\left\{\varphi^S_{R,k} : 1 \le k \le M\right\} \subset \mathrm{H}^1_S(\mathbb{R})$ with

$$\varphi^S_{R,k} = \begin{cases} \sin\left((2k-1)\pi\frac{x+R}{2R}\right), & |x| \le R \\ 0, & |x| > R \end{cases}.$$

Define $F_p\colon\ \mathrm{H}^1_S(\mathbb{R}) \to \mathrm{H}^{-1}_S(\mathbb{R})$ $(p \in [0,1])$ by

$$(F_p u)[v] = \int_{\mathbb{R}} \left[u'v' + \left(V_0 + p\int_{\mathbb{R}} \Gamma(\cdot,t)u(t)^2\,dt\right)uv - u^3 v\right]dx.$$

Start Newton method with
$p = 0$ and $u = \frac{\sqrt{2V_0}}{\cosh(\sqrt{V_0}\cdot)}$



(A1) Defectbound δ

Need a verified $\delta \geq 0$ with

$$\|F\tilde{u}\|_{H^{-1}} \leq \delta$$

Have: $\tilde{u}(x) = 0$ for $|x| > R$ and $\tilde{u}\big|_{[-R,R]} \in H^2(-R,R)$.

Thus for $\varphi \in H^1_S(\mathbb{R})$

$$(F\tilde{u})[\varphi] = \int_{-R}^{R} \left\{ \tilde{u}'\varphi' + \left[\left(V + \int_{-R}^{R} \Gamma(\cdot,t)\tilde{u}(t)^2 \, dt \right) \tilde{u} - f(\tilde{u}) \right] \varphi \right\} dx$$

(A1) Defectbound δ

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Thus for $\varphi \in \mathrm{H}^1_S(\mathbb{R})$

$$(F\tilde{u})[\varphi] = \tilde{u}'\varphi\Big|_{-R}^{R} + \int_{-R}^{R} \left[-\tilde{u}'' + \left(V + \int_{-R}^{R} \Gamma(\cdot, t)\tilde{u}(t)^2 \, dt \right)\tilde{u} - f(\tilde{u}) \right] \varphi \, dx$$

(A1) Defectbound δ

Need a verified $\delta \geq 0$ with

$$\|F\tilde{u}\|_{H^{-1}} \leq \delta$$

Have: $\tilde{u}(x) = 0$ for $|x| > R$ and $\tilde{u}\big|_{[-R,R]} \in H^2(-R,R)$.

Thus

$$\|F\tilde{u}\|_{H^{-1}} \leq \sqrt{\frac{\delta_1^2}{2\lambda} + \frac{\delta_2^2}{\sigma - \lambda^2}} =: \delta$$

- $\delta_1 := |\tilde{u}'(R)| + |\tilde{u}'(-R)|$,
- $\delta_2 := \left\| -\tilde{u}'' + \left(V + \int_{-R}^{R} \Gamma(\cdot,t)\tilde{u}(t)^2\, dt\right)\tilde{u} - f(\tilde{u})\right\|_{L^2(-R,R)}$,
- $\lambda \in (0, \sqrt{\sigma})$ arbitrary.

(A2) Norm bound for L^{-1}

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Norm bound $K \geq 0$ for L^{-1}:

$$\|u\|_{H^1} \leq K\|\Phi^{-1}Lu\|_{H^1} \quad (u \in H^1_S(\mathbb{R})). \tag{A2}$$

Spectral decomposition of $\Phi^{-1}L$ yields:

$$\text{(A2) holds} \quad \Leftrightarrow \quad \gamma := \min\{|\lambda| \colon \lambda \in \sigma(\Phi^{-1}L)\} > 0.$$

Can choose any arbitrary $K \geq \frac{1}{\gamma}$.

Compute verified lower bounds:

- $\gamma_{\text{ev}} > 0$ for $\min\{|\lambda| \colon \lambda$ isolated eigenvalue of $\Phi^{-1}L\}$,
- $\gamma_{\text{ess}} > 0$ for $\min\{|\lambda| \colon \lambda \in \sigma_{\text{ess}}(\Phi^{-1}L)\}$.

Choose

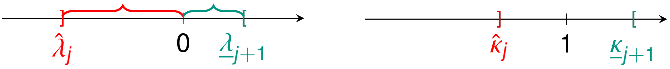
$$K = \frac{1}{\min\{\gamma_{\text{ev}}, \gamma_{\text{ess}}\}}.$$

Eigenvalue bound γ_{ev}

$$\Phi^{-1}Lu = \lambda u \underset{\kappa := \frac{1}{1-\lambda}}{\Leftrightarrow} \langle u, \varphi \rangle_{H^1} = \kappa \underbrace{(\Phi u - Lu)[\varphi]}_{=:M(u,\varphi)} \quad (\varphi \in H^1(\mathbb{R}))$$

with a symmetric and bounded bilinarform M.

Choose σ such that M is positive.



Upper eigenvalue bounds: Rayleigh-Ritz method.

Lower eigenvalue bounds: Lehmann-Goerisch and homotopy method.

Set $\gamma_{\mathrm{ev}} = \min\{|\hat{\lambda}_j|, \underline{\lambda}_{j+1}\} = \min\{|1 - \frac{1}{\hat{\kappa}_j}|, 1 - \frac{1}{\underline{\kappa}_{j+1}}\}$.

Bound for essential spectrum γ_{ess}

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Theorem (see [3])

The essential spectrum is conserved under a relatively compact perturbation.

Show: $\Phi^{-1}L$ is a relatively compact pertubation of $\Phi^{-1}L_0$ with

$$L_0 \colon \mathrm{H}^1_S(\mathbb{R}) \to \mathrm{H}^{-1}_S(\mathbb{R}), \ (L_0 u)[v] = \int_{\mathbb{R}} [u'v' + V^\infty uv] \, dx.$$

Essential spectrum of $\Phi^{-1}L_0$:

$$\sigma_{\text{ess}}(\Phi^{-1}L_0) = \left[\frac{V^\infty}{\sigma}, 1\right]$$

where $\sigma > V^\infty$ by choice of σ.

Set $\gamma_{\text{ess}} = \frac{V^\infty}{\sigma}$.

(A3)/(A4) Non-decreasing function g

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Need a non-decreasing function $g\colon [0,\infty) \to [0,\infty)$ which satisfies

$$\left\| F'(\tilde{u}+u) - F'\tilde{u} \right\|_{\mathcal{B}} \le g(\|u\|_{H^1}) \quad (u \in H^1_S(\mathbb{R})). \tag{A3}$$

and $g(t) \to 0 \ (t \to 0^+)$. (A4)

(A3)/(A4) Non-decreasing function g

Need a non-decreasing function $g\colon [0,\infty) \to [0,\infty)$ which satisfies

$$\left|\left(F'(\tilde{u}+u)v - (F'\tilde{u})v\right)[\varphi]\right| \le g(\|u\|_{H^1})\,\|v\|_{H^1}\,\|\varphi\|_{H^1} \quad (u,v,\varphi \in H^1_S(\mathbb{R})). \qquad \text{(A3)}$$

and $g(t) \to 0$ $(t \to 0^+)$. (A4)

Set

$$g(t) = \frac{3t}{2\sigma^{\frac{3}{2}}}\left(2\|\tilde{u}\|_{H^1} + t + \frac{1}{\sqrt{c}}\left(2\|\tilde{u}\|_{L^2} + \frac{t}{\sqrt{\sigma}}\right)\right).$$

Results for the one-dimensional system

Proved a non-trivial solution in the following cases:

c	V_0	σ	δ	K	α
30.0	1.0	2.133	3.085e-4	3.753	1.17e-3
40.0	1.0	1.973	3.154e-4	3.543	1.12e-3
50.0	1.0	1.866	3.174e-4	3.498	1.12e-3

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