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Computer-assisted Existence Proofs for One-dimensional Schrödinger-Poisson Systems

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Abstract

Motivated by the three-dimensional time-dependent Schrödinger-Poisson system we prove the existence of non-trivial solutions of the one-dimensional stationary Schrödinger-Poisson system using computer-assisted methods.

Starting from a numerical approximate solution, we compute a bound for its defect, and a norm bound for the inverse of the linearization at the approximate solution. For the latter, eigenvalue bounds play a crucial role, especially for the eigenvalues "close to" zero. Therefor, we use the Rayleigh-Ritz method and a corollary of the Temple-Lehmann Theorem to get enclosures of the crucial eigenvalues of the linearization below the essential spectrum.

With these data in hand, we can use a fixed-point argument to obtain the desired existence of a non-trivial solution "nearby" the approximate one. In addition to the pure existence result, the used methods also provide an enclosure of the exact solution.

Keywords: computer-assisted proof, existence, enclosure, Schrödinger-Poisson system

1 Introduction and Basic Notations

Motivated by the three-dimensional time-dependent Schrödinger-Poisson system appearing in quantum mechanics, more precisely in modeling effects occurring in todays semiconductor technology, we are interested in non-trivial solutions of the time-independent stationary system

$$\left.\begin{aligned} -\Delta v + (V+\phi_v)v &= f(v) \\ -\Delta \phi_v &= v^2 \end{aligned}\right\} \text{ on } \mathbb{R}^3, \quad \lim_{|x|\to\infty} v(x) = 0, \quad \lim_{|x|\to\infty} \phi_v(x) = 0 \tag{1}$$

considered in many papers, e.g. [2], [13] and [6], where (1) can be derived from the time-dependent system via a standing wave ansatz if the non-linearity satisfies $f(e^{\mathrm{i}\varphi}z) = e^{\mathrm{i}\varphi}f(z)$ for all $z \in \mathbb{C}, \varphi \in \mathbb{R}$. More details about the physical background are to be found in [9].

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In [5] and [6], the energy functional associated with (1) is minimized over the Nehari manifold to prove existence of positive solutions of (1) (with $V = 0$, $f(v) = |v|^{p-1}v$ for some ranges of p). In [13] the author derives ranges for p in which positive radially symmetric solutions of (1) with $V = 1$ do exist or not, i.e. for $p \in (1, 2]$ no positive radial solution exists and for $p \in (2, 5)$ (including the case $p = 3$) there is a positive radial solution. Moreover, in [5] non-existence results for $p \leq 1$ and $p \geq 5$ are proved by using suitable Pohozaev identities. Multiplicity results in a radially symmetric setting can be found in [1]. In [15] the authors use variational methods and morse theory to prove existence of multiple non-trivial solutions of (1) if the potential V is continuous and bounded from below and the non-linearity f satisfies the growth condition $|f(x, v)| \leq const \cdot (1 + |v|^p)$, where $p \in (1, 5)$.

As a test problem for computer-assisted proofs we consider the one-dimensional stationary Schrödinger-Poisson system

$$\left.\begin{aligned} -u'' + (V + \phi_u)u &= u^3 \\ -\phi_u'' + c\phi_u &= u^2 \end{aligned}\right\} \text{ on } \mathbb{R}, \quad \lim_{x \to \pm\infty} u(x) = 0, \quad \lim_{x \to \pm\infty} \phi_u(x) = 0, \tag{2}$$

where V is a positive and constant potential and $c > 0$.

To prove non-trivial solutions of (2) we first "solve" the second equation using the corresponding Green's function $\Gamma \colon \mathbb{R} \to \mathbb{R}$, $\Gamma(x) := \frac{1}{2\sqrt{c}} \exp(-\sqrt{c}|x|)$, and insert the result into the first one:

$$-u'' + (V + \Gamma * u^2)u = u^3. \tag{3}$$

The second order problem (3), with the boundary condition $u(x) \to 0$ as $x \to \pm\infty$ modelled in an appropriate way, will be formulated weakly in the H^1-space of symmetric functions $H_s^1(\mathbb{R}) := \{u \in H^1(\mathbb{R}) \colon u(x) = u(-x) \text{ for a.e. } x \in \mathbb{R}\}$ endowed with the inner product

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

where $\langle \cdot, \cdot \rangle_{L^2}$ denotes the usual inner product on $L^2(\mathbb{R})$ and $\sigma > 0$ is a constant to be specified later (see Subsection 2.3).

The weak formulation of problem (2) respectively (3) now reads:
Find $u \in H_s^1(\mathbb{R})$ such that

$$\int_{\mathbb{R}} u'\varphi' \, dx + \int_{\mathbb{R}} \left(V + (\Gamma * u^2)\right) u\varphi \, dx = \int_{\mathbb{R}} u^3 \varphi \, dx \quad \text{for all } \varphi \in H_s^1(\mathbb{R}). \tag{4}$$

Moreover, we will need the topological dual space of $H_s^1(\mathbb{R})$ denoted by $H_s^{-1}(\mathbb{R})$, which will be endowed with the usual dual norm $\|\cdot\|_{H^{-1}}$. Functions $u \in L_s^2(\mathbb{R}) := \{u \in L^2(\mathbb{R}) \colon u(x) = u(-x) \text{ for a.e. } x \in \mathbb{R}\}$ can be identified with elements in $H_s^{-1}(\mathbb{R})$ via

$$u[\varphi] := \int_{\mathbb{R}} u\varphi \, dx \quad \text{for all } \varphi \in H_s^1(\mathbb{R})$$

and we define their first derivative $u' \in H_s^{-1}(\mathbb{R})$ by

$$u'[\varphi] := -\int_{\mathbb{R}} u\varphi' \, dx \quad \text{for all } \varphi \in H_s^1(\mathbb{R}).$$

Riesz' Representation Lemma for bounded linear functionals implies that

$$\Phi\colon H_s^1(\mathbb{R}) \to H_s^{-1}(\mathbb{R}),\ \Phi(u) := -u'' + \sigma u, \tag{5}$$

i.e. $(\Phi u)[\varphi] = \langle u, \varphi \rangle_{H^1}$ for all $u, \varphi \in H_s^1(\mathbb{R})$, defines an isometric isomorphism.

Since the proof of the central Theorem 1 is based on a zero finding problem formulation of (4), we define the operator

$$F\colon H_s^1(\mathbb{R}) \to H_s^{-1}(\mathbb{R}),\ Fu := -u'' + (V + \Gamma * u^2 - u^2)u, \tag{6}$$

i.e. $(Fu)[\varphi] = \int_{\mathbb{R}} \left[u'\varphi' + (V + \Gamma * u^2 - u^2)u\varphi \right] dx$. Obviously, $u \in H_s^1(\mathbb{R})$ solves $Fu = 0$ if and only if u solves (4).

Moreover, let $L\colon H_s^1(\mathbb{R}) \to H_s^{-1}(\mathbb{R})$ denote the linearization of F at ω, i.e.

$$Lu := (F'\omega)(u) = -u'' + (V + \Gamma * \omega^2 - 3\omega^2)u + 2(\Gamma * (\omega u))\omega. \tag{7}$$

Hence, we get $(Lu)[\varphi] = \int_{\mathbb{R}} \left[u'\varphi' + (V + \Gamma * \omega^2 - 3\omega^2)u\varphi + 2(\Gamma * (\omega u))\omega\varphi \right] dx$.

To improve readability of the proof of Theorem 1, some of the technical estimates needed are discussed in advance in the subsequent Proposition.

Proposition 1. *The following identity and inequalities hold true:*

(a) $\|u\|_{L^2} \le \frac{1}{\sqrt{\sigma}} \|u\|_{H^1}$ *for all* $u \in H_s^1(\mathbb{R})$,

(b) $\|u\|_{H^{-1}} \le \frac{1}{\sqrt{\sigma}} \|u\|_{L^2}$ *for all* $u \in L_s^2(\mathbb{R})$,

(c) $\|u\|_\infty \le \sqrt{\|u\|_{L^2} \|u'\|_{L^2}} \le \frac{1}{\sqrt{2}\sigma^{\frac{1}{4}}} \|u\|_{H^1}$ *for all* $u \in H_s^1(\mathbb{R})$,

(d) $F(\omega + v) - F(\omega + w) - L(v - w) = -\left[(\omega + v)^3 - (\omega + w)^3 - 3\omega^2(v - w) \right]$ $+(\Gamma*(\omega+v)^2)(\omega+v) - (\Gamma*(\omega+w)^2)(\omega+w) - (\Gamma*\omega^2)(v-w) - 2(\Gamma*(\omega(v-w)))$ *for all* $\omega, v, w \in H_s^1(\mathbb{R})$,

(e) $\left\| (\omega + v)^3 - (\omega + w)^3 - 3\omega^2(v - w) \right\|_{H^{-1}} \le$ $\frac{\|v-w\|_{H^1}}{2\sigma^{\frac{3}{2}}} \left[3\|\omega\|_{H^1} (\|v\|_{H^1} + \|w\|_{H^1}) + \|v\|_{H^1}^2 + \|v\|_{H^1} \|w\|_{H^1} + \|w\|_{H^1}^2 \right]$ *for all* $\omega, v, w \in H_s^1(\mathbb{R})$,

(f) $\big\| (\Gamma * (\omega + v)^2)(\omega + v) - (\Gamma * (\omega + w)^2)(\omega + w)$ $-(\Gamma * \omega^2)(v - w) - 2(\Gamma * (\omega(v - w)))\omega \big\|_{H^{-1}} \le$ $\frac{\|v-w\|_{H^1}}{2\sqrt{c}\sigma^{\frac{3}{2}}} \left[3\|\omega\|_{L^2} (\|v\|_{H^1} + \|w\|_{H^1}) + \frac{1}{\sqrt{\sigma}} (\|v\|_{H^1}^2 + \|v\|_{H^1} \|w\|_{H^1} + \|w\|_{H^1}^2) \right]$ *for all* $\omega, v, w \in H_s^1(\mathbb{R})$.

Proof. (a) Since σ is positive, we obtain

$$\|u\|_{L^2}^2 \leq \frac{1}{\sigma}\|u'\|_{L^2}^2 + \|u\|_{L^2}^2 = \frac{1}{\sigma}\|u\|_{H^1}^2 .$$

(b) Using Cauchy-Schwarz' inequality, (b) follows from (a) by the dual estimate:

$$\|u\|_{H^{-1}} = \sup_{\substack{\varphi\in H_s^1(\mathbb{R})\\ \|\varphi\|_{H^1}=1}} \left|\int_{\mathbb{R}} u\varphi\ dx\right| \leq \sup_{\substack{\varphi\in H_s^1(\mathbb{R})\\ \|\varphi\|_{H^1}=1}} \|u\|_{L^2}\|\varphi\|_{L^2} \leq \frac{1}{\sqrt{\sigma}}\|u\|_{L^2} .$$

(c) By Sobolev's Embedding Theorem $H^1(\mathbb{R})$ embeds continuously into the space of bounded continuous functions on $\mathbb{R}$ endowed with the usual sup-norm $\|\cdot\|_\infty$. Thus, we only have to verify the asserted embedding constant.

First, for fixed $x \in \mathbb{R}$, we get

$$\begin{aligned} u(x)^2 &= 2\int_{-\infty}^{x} uu'\ dx \leq 2\int_{-\infty}^{x} |uu'|\ dx, \\ u(x)^2 &= -2\int_{x}^{\infty} uu'\ dx \leq 2\int_{x}^{\infty} |uu'|\ dx. \end{aligned}$$

Adding both estimates and applying Cauchy-Schwarz' inequality we obtain

$$u(x)^2 = \int_{\mathbb{R}} |uu'|\ dx \leq \|u\|_{L^2}\|u'\|_{L^2} .$$

Taking the supremum over x yields $\|u\|_\infty^2 \leq \|u\|_{L^2}\|u'\|_{L^2}$ and thus, applying Young's inequality,

$$\|u\|_\infty^2 \leq \frac{1}{2}\left(\frac{\|u'\|_{L^2}^2}{\sqrt{\sigma}} + \sqrt{\sigma}\|u\|_{L^2}^2\right) = \frac{1}{2\sqrt{\sigma}}\|u\|_{H^1}^2 .$$

(d) Using the definitions of F and L respectively we obtain

$$\begin{aligned} &F(\omega+v) - F(\omega+w) - L(v-w) \\ &\quad= -(\omega+v)'' + (V + \Gamma*(\omega+v)^2 - (\omega+v)^2)(\omega+v) \\ &\qquad - \left[-(\omega+w)'' + (V+\Gamma*(\omega+w)^2 - (\omega+w)^2)(\omega+w)\right] \\ &\qquad - \left[-(v-w)'' + (V+\Gamma*\omega^2 - 3\omega^2)(v-w) + 2(\Gamma*(\omega(v-w)))\omega\right] \\ &\quad= -\left[(\omega+v)^3 - (\omega+w)^3 - 3\omega^2(v-w)\right] \\ &\qquad + (\Gamma*(\omega+v)^2)(\omega+v) - (\Gamma*(\omega+w)^2)(\omega+w) \\ &\qquad - (\Gamma*\omega^2)(v-w) - 2(\Gamma*(\omega(v-w))). \end{aligned}$$

(e) We note that

$$(\omega+v)^3-(\omega+w)^3-3\omega^2(v-w) = 3\int_0^1 \left[(\omega+tv+(1-t)w)^2-\omega^2\right](v-w)\,dt.$$

Multiplying by a test function, integrating over $\mathbb{R}$ and exchanging the order of integration yields, together with (a) and (c),

$$\begin{aligned}
&\left\|(\omega+v)^3-(\omega+w)^3-3\omega^2(v-w)\right\|_{H^{-1}} \\
&\le 3 \sup_{\substack{\varphi\in H_s^1(\mathbb{R})\\ \|\varphi\|_{H^1}=1}} \int_0^1 \left|\int_{\mathbb{R}} \left[(\omega+tv+(1-t)w)^2-\omega^2\right](v-w)\varphi\,dx\right| dt \\
&\le \frac{3}{\sigma}\|v-w\|_{H^1}\int_0^1 \left\|(\omega+tv+(1-t)w)^2-\omega^2\right\|_\infty dt \\
&\le \frac{1}{2\sigma^{\frac{3}{2}}}\|v-w\|_{H^1}\Big[3\|\omega\|_{H^1}(\|v\|_{H^1}+\|w\|_{H^1}) \\
&\quad + \|v\|_{H^1}^2+\|v\|_{H^1}\|w\|_{H^1}+\|w\|_{H^1}^2\Big].
\end{aligned}$$

(f) Since Γ is bounded by $\frac{1}{2\sqrt{c}}$, Cauchy-Schwarz' inequality and (a) yield

$$\begin{aligned}
\int_{\mathbb{R}}(\Gamma*(u_1u_2))u_3\varphi\,dx &\le \|\Gamma\|_\infty\left(\int_{\mathbb{R}}u_1u_2\,dy\right)\left(\int_{\mathbb{R}}u_3\varphi\,dx\right) \\
&\le \frac{1}{2\sqrt{c\sigma}}\|u_1\|_{L^2}\|u_2\|_{L^2}\|u_3\|_{L^2}\|\varphi\|_{H^1}
\end{aligned}$$

for $u_1,u_2,u_3,\varphi\in H_s^1(\mathbb{R})$. Using this inequality together with similar arguments as in (e), we obtain

$$\begin{aligned}
&\Big\|(\Gamma*(\omega+v)^2)(\omega+v)-(\Gamma*(\omega+w)^2)(\omega+w) \\
&\qquad -(\Gamma*\omega^2)(v-w)-2(\Gamma*(\omega(v-w)))\omega\Big\|_{H^{-1}} \\
&\le \sup_{\substack{\varphi\in H_s^1(\mathbb{R})\\ \|\varphi\|_{H^1}=1}} \int_0^1 \left|\int_{\mathbb{R}}\Big[\big(\Gamma*((\omega+tv+(1-t)w)^2-\omega^2)\big)(v-w)\varphi\right. \\
&\quad +2\big(\Gamma*((\omega+tv+(1-t)w)(v-w))\big)(tv+(1-t)w)\varphi \\
&\quad \left.-2\big(\Gamma*(tv+(1-t)w)(v-w)\big)\omega\varphi\Big]\,dx\right|dt \\
&\le \frac{1}{2\sqrt{c\sigma}}\|v-w\|_{H^1}\int_0^1\big[6\|\omega\|_{L^2}\|tv+(1-t)w\|_{L^2} \\
&\quad +3\|tv+(1-t)w\|_{L^2}^2\big]\,dt \\
&\le \frac{1}{2\sqrt{c}\sigma^{\frac{3}{2}}}\|v-w\|_{H^1}\Big[3\|\omega\|_{L^2}(\|v\|_{H^1}+\|w\|_{H^1}) \\
&\quad +\frac{1}{\sqrt{\sigma}}(\|v\|_{H^1}^2+\|v\|_{H^1}\|w\|_{H^1}+\|w\|_{H^1}^2)\Big].
\end{aligned}$$

□

2 Existence and Enclosure Theorem

In this section we will describe the main steps of our computer-assisted existence proof for the Schrödinger-Poisson system (2), or (4) respectively. Essentially we follow the lines in [4], [11] and [10]. What is new here is the non-locality of the Schrödinger-Poisson problem (cf. (3)) which requires new techniques for the computation of the defect bound and the eigenvalue bounds addressed below. We also refer to [17], where several issues studied here had been addressed already.

First, let $\omega \in H_s^1(\mathbb{R})$ be an approximate solution of (4) of the following form:

$$\omega = \begin{cases} \omega_0, & \text{in } (-R, R), \\ 0, & \text{in } \mathbb{R} \setminus (-R, R), \end{cases} \tag{8}$$

for some suitable $R > 0$ and symmetric $\omega_0 \in H_0^1(-R, R)$. Hence, ω has compact support in $[-R, R]$. We note that (8) is no strong restriction on the numerical method used to compute ω, since most of the common methods yield a compact supported approximate solution anyway. Moreover, we note that ω can be computed via usual (i.e. non-verified) numerical algorithms, e.g. a Newton method (see Subsection 2.1). We only have to make sure that the numerical method used yields an approximate solution in the space $H_s^1(\mathbb{R})$.

The following central Theorem 1 requires the computation of the following two crucial constants which will be addressed in Subsection 2.2 and 2.3 below.

(a) Suppose a bound $\delta \geq 0$ for the defect (residual) of ω has been computed, i.e.

$$\|F\omega\|_{H^{-1}} = \left\|-\omega'' + (V + \Gamma * \omega^2 - \omega^2)\omega\right\|_{H^{-1}} \leq \delta. \tag{9}$$

(b) Assume a constant $K \geq 0$ is in hand such that

$$\|u\|_{H^1} \leq K \|Lu\|_{H^{-1}} \quad \text{for all } u \in H_s^1(\mathbb{R}) \tag{10}$$

with L defined in (7).

We note that K satisfying (10) is actually a norm bound for the inverse of L. For the computation of K a substantial use of computer-assisted methods is needed. A manner of computing such constants δ and K will be described in Subsections 2.2 and 2.3.

Theorem 1. *Suppose some $\alpha \geq 0$ exists such that*

$$\delta \leq \frac{\alpha}{K} - \frac{\alpha^2}{2\sigma^{\frac{3}{2}}} \left(3\|\omega\|_{H^1} + \alpha + \frac{1}{\sqrt{c}}\left(3\|\omega\|_{L^2} + \frac{\alpha}{\sqrt{\sigma}}\right)\right) \tag{11}$$

and

$$K \cdot \frac{3\alpha}{2\sigma^{\frac{3}{2}}} \left(2\|\omega\|_{H^1} + \alpha + \frac{1}{\sqrt{c}}\left(2\|\omega\|_{L^2} + \frac{\alpha}{\sqrt{\sigma}}\right)\right) < 1. \tag{12}$$

Then there exists an exact solution $u^* \in H_s^1(\mathbb{R})$ of the Schrödinger-Poisson system (2), *or* (4) *respectively, satisfying the enclosure*

$$\|u^* - \omega\|_{H^1} \leq \alpha.$$

Proof (see proof of Theorem 1 in [11]). Clearly, L is bounded and, due to assumption (10), one-to-one. Next, we will prove that L is onto as well. Therefor, we first show that the range of L is closed. So let $(u_n)_n$ be a sequence in $H^1_s(\mathbb{R})$ and $w \in H^{-1}_s(\mathbb{R})$ such that $Lu_n \to w$ as $n \to \infty$ in $H^{-1}_s(\mathbb{R})$. Since $(Lu_n)_n$ is a Cauchy sequence, by (10), $(u_n)_n$ is a Cauchy sequence in $H^1_s(\mathbb{R})$ converging to some $u \in H^1_s(\mathbb{R})$. By the boundedness of L we obtain $Lu_n \to Lu$ as $n \to \infty$ in $H^{-1}_s(\mathbb{R})$ and hence $Lu = w$, i.e. the range is closed.

It remains to show that the range of L is dense in $H^{-1}_s(\mathbb{R})$. Since Φ is an isometric isomorphism it is equivalent to show that $\{\Phi^{-1}L\varphi \colon \varphi \in H^1_s(\mathbb{R})\}$ is dense in $H^1_s(\mathbb{R})$. Now, let $u \in H^1_s(\mathbb{R})$ be an element of its orthogonal complement, i.e.

$$\left\langle u, \Phi^{-1}L\varphi \right\rangle_{H^1} = 0 \qquad \text{for all } \varphi \in H^1_s(\mathbb{R}).$$

Using (5), we obtain $\left\langle u, \Phi^{-1}L\varphi \right\rangle_{H^1} = (L\varphi)[u]$, and hence by Fubini's Theorem we obtain

$$\begin{aligned} 0 = (L\varphi)[u] &= \int_{\mathbb{R}} \big[\varphi' u' + (V + \Gamma * \omega^2 - 3\omega^2)\varphi u + 2(\Gamma * (\omega\varphi))\omega u\big]\, dx \\ &= \int_{\mathbb{R}} \big[u'\varphi' + (V + \Gamma * \omega^2 - 3\omega^2)u\varphi + 2(\Gamma * (\omega u))\omega\varphi\big]\, dx = (Lu)[\varphi] \end{aligned}$$

for all $\varphi \in H^1_s(\mathbb{R})$, implying $Lu = 0$. Therefore, applying (10), we get $u = 0$ deducing the asserted density and thus, proving that L is onto. Altogether, L is bijective.

Introducing the error $v := u - \omega$, problem (4) is equivalent to the fixed-point equation

$$\begin{aligned} v = -L^{-1}\big[&- \omega'' + (V + \Gamma * \omega^2 - \omega^2)\omega - \big((\omega + v)^3 - \omega^3 - 3\omega^2 v\big) \\ &+ (\Gamma * (\omega + v)^2)(\omega + v) - (\Gamma * \omega^2)(\omega + v) - 2(\Gamma * (\omega v))\omega\big] =: Tv, \end{aligned} \tag{13}$$

where the right-hand-side defines a fixed point operator $T \colon H^1_s(\mathbb{R}) \to H^1_s(\mathbb{R})$ (cf. (19) in [11]). Let $\mathcal{V} := \{v \in H^1_s(\mathbb{R}) \colon \|v\|_{H^1} \le \alpha\}$ with α satisfying (11) and (12). Using (13) and (10), (9), Proposition 1 (e) and (f) (with $w = 0$), and (11) we obtain for $v \in \mathcal{V}$:

$$\begin{aligned} \|Tv\|_{H^1} \le K\big[&\left\|-\omega'' + (V + \Gamma * \omega^2 - \omega^2)\omega\right\|_{H^{-1}} + \left\|\big((\omega + v)^3 - \omega^3 - 3\omega^2 v\big)\right\|_{H^{-1}} \\ &+ \left\|(\Gamma * (\omega + v)^2)(\omega + v) - (\Gamma * \omega^2)(\omega + v) - 2(\Gamma * (\omega v))\omega\right\|_{H^{-1}} \big] \\ \le K &\left[\delta + \frac{\|v\|^2_{H^1}}{2\sigma^{\frac{3}{2}}}\left(3\|\omega\|_{H^1} + \|v\|_{H^1} + \frac{1}{\sqrt{c}}\left(3\|\omega\|_{L^2} + \frac{\|v\|_{H^1}}{\sqrt{\sigma}}\right)\right)\right] \\ \le K &\left[\delta + \frac{\alpha^2}{2\sigma^{\frac{3}{2}}}\left(3\|\omega\|_{H^1} + \alpha + \frac{1}{\sqrt{c}}\left(3\|\omega\|_{L^2} + \frac{\alpha}{\sqrt{\sigma}}\right)\right)\right] \le \alpha, \end{aligned}$$

implying $T(\mathcal{V}) \subseteq \mathcal{V}$. Moreover, by (13) and (10), Proposition 1 (e) and (f) we deduce for $v, w \in \mathcal{V}$:

$$
\begin{aligned}
\|Tv - Tw\|_{H^{-1}} \le K \big[& \big\|(\omega+v)^3 - (\omega+w)^3 - 3\omega^2(v-w)\big\|_{H^{-1}} \\
& + \big\|(\Gamma * (\omega+v)^2)(\omega+v) - (\Gamma * (\omega+w)^2)(\omega+w) \\
& - (\Gamma * \omega^2)(v-w) - 2(\Gamma * (\omega(v-w)))\omega\big\|_{H^{-1}} \\
\le K & \frac{3\alpha}{2\sigma^{\frac{3}{2}}} \left(2\|\omega\|_{H^1} + \alpha + \frac{1}{\sqrt{c}} \left(2\|\omega\|_{L^2} + \frac{\alpha}{\sqrt{\sigma}} \right) \right) \|v-w\|_{H^1},
\end{aligned}
$$

and hence, by (12), T is a contraction on $\mathcal{V}$. Therefore, Banach's Fixed-Point Theorem yields a fixed point $v^* \in \mathcal{V}$ of T and thus, $u^* := \omega + v^*$ is a solution of problem (2), or (4) respectively. Moreover, u^* satisfies the asserted rigorous error estimate $\|u^* - \omega\|_{H^1} = \|v^*\|_{H^1} \le \alpha$. □

Remark 1. (a) Since we are interested in non-trivial solutions of (4), we additionally have to check that $\|\omega\|_{H^1}$ is strictly larger then α, since otherwise the solution u^* provided by Theorem 1 could be the trivial one.

(b) Using Proposition 1 (a) and (c) respectively, we also get the following error bounds:

$$
\|u^* - \omega\|_{L^2} \le \frac{\alpha}{\sqrt{\sigma}} \quad \text{and} \quad \|u^* - \omega\|_\infty \le \frac{\alpha}{\sqrt{2}\sigma^{\frac{1}{4}}}.
$$

(c) Suppose (10) is satisfied for some K which is not too "large", i.e. L is not close to being non-invertible. Then assumptions (11) and (12) hold true for some "small" α if δ is sufficiently small. Hence, by (9), condition (11) is a demand on the accuracy of the approximate solution ω (measured by its residual).

To get a better understanding, let $h\colon [0,\infty) \to \mathbb{R}$ be defined by the right-hand-side of (11), i.e.

$$
h(t) := \frac{t}{K} - \frac{t^2}{2\sigma^{\frac{3}{2}}} \left(3\|\omega\|_{H^1} + t + \frac{1}{\sqrt{c}} \left(3\|\omega\|_{L^2} + \frac{t}{\sqrt{\sigma}} \right) \right) \quad \text{for all } t \in [0,\infty).
$$

Obviously, condition (11) is satisfiable if and only if the defect bound δ is less or equal to $\delta_{\max} := \max\{h(t)\colon t \in [0,\infty)\}$. In the affirmative case α can be choosen between some values $\alpha_{\min}$ and $\alpha_{\max}$ (see Figure 1). Since we are interested in a small error bound, we select α close to $\alpha_{\min}$. A possible procedure to compute α is described in Remark 2 (b) in [4].

2.1 Computation of an approximate solution ω

We compute an approximate solution ω of (4) in the finite dimensional subspace $V_M := \operatorname{span}\{\phi_k\colon k = 1,\dots,M\} \subseteq H_s^1(\mathbb{R})$, where

$$
\phi_k\colon \mathbb{R} \to \mathbb{R},\ \phi_k(x) := \begin{cases} \sin\left((2k-1)\pi\frac{x+R}{2R}\right), & |x| \le R, \\ 0, & |x| > R, \end{cases}
$$

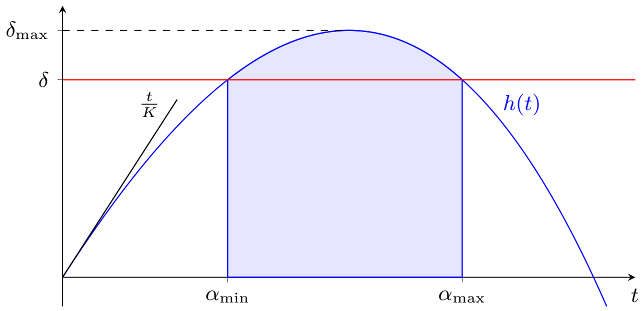

Figure 1: Possible choices of α

with $R > 0$ chosen suitably to obtain an error bound as small as possible. More details about the choice of R are mentioned in Subsection 2.2.

To calculate ω we consider the operator family

$$F_p\colon H_s^1(\mathbb{R}) \to H_s^{-1}(\mathbb{R}),\ F_p(u) := -u'' + (V + p(\Gamma * u^2) - u^2)u$$

parametrized by $p \in [0,1]$. Clearly, $u \in H_s^1(\mathbb{R})$ solves (4) if and only if $F_1(u) = 0$ (cf. (6)), i.e. we can compute $\omega \in H_s^1(\mathbb{R})$ satisfying $F_1(\omega) \approx 0$ via a Newton iteration.

First, we note that $u_0(x) = \sqrt{2V}/\cosh(\sqrt{V}x)$ for all $x \in \mathbb{R}$ solves $F_0(u) = 0$ exactly. Thus, we compute an approximation $\omega_0^{(0)} \in V_M$ using a least squares method. Starting a Newton iteration (for the problem $F_0(u) = 0$) at $\omega_0^{(0)}$, we obtain improved approximations $\omega_0^{(1)}, \omega_0^{(2)}, \ldots$, and stop this iteration at some index n_0 where $F_0(\omega_0^{(n_0)})$ is below some prescribed tolerance.

Next, we perform the usual path following algorithm, i.e. we increase p in small steps (up to $p = 1$) by a step size δ_p, where $\delta_p = 0.5$ turned out to be sufficient in all our applications. Here, to compute an approximate solution of $F_{p+\delta_p}(u) = 0$, we start a Newton's method at $\omega_{p+\delta_p}^{(0)} := \omega_p^{(n_p)}$, with $\omega_p^{(n_p)}$ denoting the final approximate solution of the previous problem $F_p(u) = 0$. Finally, when p is equal to 1, we get an approximate solution $\omega \in H_s^1(\mathbb{R})$ with $F_1(\omega) \approx 0$.

As mentioned earlier, non of those Newton iterations has to be done using verified numerics, i.e. no errors need to be taken into account at this stage. Thus, it is sufficient to use (non-verified) quadrature formulas to compute the integrals needed in the Newton steps. In all our numerical examples the chained Simpson's rule is used. More details about the choice of R and M can be found in Section 3.

2.2 Computation of the defect bound δ

In contrast to the determination of ω, in the context of the defect bound all errors have to be taken into account using interval methods, e.g. INTLAB (see [14]). Obviously, ω, computed by the method described in Subsection 2.1, is a function in $H^2(-R,R)$ after restriction to $(-R,R)$. Thus, using integration by parts and Proposition 1 (c) and Cauchy-Schwarz' inequality (with some $\eta>0$), we get for all $\varphi\in H^1_s(\mathbb{R})$:

$$\begin{aligned}
&\left|\int_{\mathbb{R}}\left[\omega'\varphi'+(V+\Gamma*\omega^2-\omega^2)\omega\varphi\right]\,dx\right|\\
&\quad\le\left|\omega'\varphi\big|_{-R}^{R}\right|+\int_{-R}^{R}\left|\left[-\omega''+(V+\Gamma*\omega^2-\omega^2)\omega\right]\varphi\right|dx\\
&\quad\le\delta_1\sqrt{\|\varphi\|_{L^2}\|\varphi'\|_{L^2}}+\delta_2\|\varphi\|_{L^2}\\
&\quad\le\left(\delta_1^2+\frac{\delta_2^2}{\eta}\right)^{\frac12}\left(\|\varphi\|_{L^2}\|\varphi'\|_{L^2}+\eta\|\varphi\|_{L^2}^2\right)^{\frac12}
\end{aligned}$$

with $\delta_1:=|\omega'(R)|+|\omega'(-R)|$ and $\delta_2:=\left\|-\omega''+(V+\Gamma*\omega^2-\omega^2)\omega\right\|_{L^2(-R,R)}$.

Applying Young's inequality gives $\|\varphi\|_{L^2}\|\varphi'\|_{L^2}\le\frac{1}{2\lambda}(\|\varphi'\|_{L^2}^2+\lambda^2\|\varphi\|_{L^2}^2)$ for any $\lambda>0$. Choosing $\lambda<\sqrt{\sigma}$ and $\eta:=\frac{\sigma-\lambda^2}{2\lambda}$, we obtain

$$\begin{aligned}
&\left\|-\omega''+(V+\Gamma*\omega^2-\omega^2)\omega\right\|_{H^{-1}}\\
&\quad\le\sup_{\substack{\varphi\in H^1_s(\mathbb{R})\\ \|\varphi\|_{H^1}=1}}\left(\frac{1}{2\lambda}\left(\delta_1^2+\frac{\delta_2^2}{\eta}\right)\right)^{\frac12}\left(\|\varphi'\|_{L^2}^2+\left(\lambda^2+2\eta\lambda\right)\|\varphi\|_{L^2}^2\right)^{\frac12}\\
&\quad=\sup_{\substack{\varphi\in H^1_s(\mathbb{R})\\ \|\varphi\|_{H^1}=1}}\left(\frac{1}{2\lambda}\left(\delta_1^2+\frac{\delta_2^2}{\eta}\right)\right)^{\frac12}\|\varphi\|_{H^1}=\left(\frac{{\delta_1}^2}{2\lambda}+\frac{{\delta_2}^2}{\sigma-\lambda^2}\right)^{\frac12}=:\delta.
\end{aligned}$$

Therefore, the computation of δ requires a rigorous evaluation of ω' at $\pm R$ (for computing δ_1) and a verified computation of an integral (for obtaining δ_2) which can be done by quadrature formulas with verified remainder term bounds, or explicitly (as in our case). Finally, we can (approximately) minimize over all possible λ to obtain a defect bound as small as possible.

We close this subsection by giving a short remark on the choice of R. Since we expect the solution of (4) to decay "fast" for $|x|$ large, δ_1 becomes "small" if R is chosen sufficiently "large". However, a "moderate" R is needed to minimize the computational effort for the computation of δ_2 and K. Hence, we need to balance both effects.

2.3 Computation of the norm bound K

Using the isometric isomorphism Φ defined in (5), we get $\|Lu\|_{H^{-1}}=\left\|\Phi^{-1}Lu\right\|_{H^1}$ for all $u\in H^1_s(\mathbb{R})$. Since $\Phi^{-1}L$ is symmetric with respect to the inner product $\langle\cdot,\cdot\rangle_{H^1}$ and defined on the whole space $H^1_s(\mathbb{R})$, $\Phi^{-1}L$ is selfadjont. The spectral decomposition of $\Phi^{-1}L$ implies that assumption (10) holds true if and only if

$$k:=\min\{|\lambda|\colon\lambda\text{ is in the spectrum of }\Phi^{-1}L\}>0,\tag{14}$$

and in the affirmative case is satisfied for any $K \geq \frac{1}{k}$.

Thus, the remaining task is the computation of a positive lower bound for the spectrum of $\Phi^{-1}L$ (implying (14)). We divide the computation into two steps: First, we compute the essential spectrum σ_{ess} of $\Phi^{-1}L$. The second step treats the remaining part of the spectrum, i.e. the isolated eigenvalues of finite multiplicity.

Essential spectrum

Proposition 2.

$$\sigma_{ess} = \left[\min\left\{1, \frac{V}{\sigma}\right\}, \max\left\{1, \frac{V}{\sigma}\right\}\right] =: I.$$

Proof. As a first step, we show that $\Phi^{-1}L$ is a compact perturbation of $\Phi^{-1}L_0$ with

$$L_0\colon H^1_s(\mathbb{R}) \to H^{-1}_s(\mathbb{R}),\ L_0 u := -u'' + Vu.$$

Let $(u_n)_n$ be a bounded sequence in $H^1_s(\mathbb{R})$ and $\varepsilon > 0$. Since ω is of the form (8), i.e. ω has compact support, we obtain for all $|x| \geq R$:

$$(\Gamma * \omega^2)(x) = \frac{e^{-\sqrt{c}|x|}}{2\sqrt{c}} \int_{-R}^{R} e^{\mathrm{sign}(x)\sqrt{c}y} \omega(y)^2\,dy \to 0 \quad \text{as } x \to \pm\infty. \tag{15}$$

Using Proposition 1 (a) we note that $(u_n)_n$ is a bounded sequence in $L^2_s(\mathbb{R})$ and thus, using (15), there exists $\tilde{R} \geq R$ such that

$$\left\|(\Gamma * \omega^2)(u_n - u_m)\right\|_{L^2(\{|x|>\tilde{R}\})} \leq \sup_{\{|x|>\tilde{R}\}} |(\Gamma * \omega^2)(x)| \underbrace{\|u_n - u_m\|_{L^2}}_{\leq C} \leq \frac{\varepsilon}{6} \tag{16}$$

(with C independent of n and m).

Since $(u_n)_n$ is also bounded in $H^1_s(-\tilde{R}, \tilde{R})$, Sobolev-Kondrachev-Rellich's Embedding Theorem yields a subsequence $(u_{n_k})_k$ converging in $L^2_s(-\tilde{R}, \tilde{R})$. Thus, we find $\tilde{l} \in \mathbb{N}$ such that

$$\left\|3\omega^2(u_{n_k} - u_{n_l})\right\|_{L^2} = \left\|3\omega^2(u_{n_k} - u_{n_l})\right\|_{L^2(-\tilde{R},\tilde{R})} \leq \frac{\varepsilon}{3} \quad \text{for all } k, l \geq \tilde{l},$$

and (using (16) and the boundedness of $(u_{n_k})_k$)

$$\left\|(\Gamma * \omega^2)(u_{n_k} - u_{n_l})\right\|_{L^2} \leq \frac{\varepsilon}{3} \quad \text{and} \quad \|(\Gamma * (\omega(u_{n_k} - u_{n_l})))\omega\|_{L^2} \leq \frac{\varepsilon}{6}$$

for all $k, l \geq \tilde{l}$, where the second term is treated similarly to the first one.

Summing up, we obtain

$$\begin{aligned}\|(L - L_0)(u_{n_k} - u_{n_l})\|_{L^2} \leq{}& \left\|3\omega^2(u_{n_k} - u_{n_l})\right\|_{L^2} + \left\|(\Gamma * \omega^2)(u_{n_k} - u_{n_l})\right\|_{L^2} \\ &+ 2\,\|(\Gamma * (\omega(u_{n_k} - u_{n_l})))\omega\|_{L^2} \leq \varepsilon\end{aligned}$$

for all $k, l \geq \tilde{l}$. Therefore, $((L - L_0)u_{n_k})_k$ is a Cauchy sequence in $L_s^2(\mathbb{R})$ and thus, convergent in $L_s^2(\mathbb{R})$ and, by Proposition 1 (b), convergent in $H_s^{-1}(\mathbb{R})$. Since Φ is an isometric isomorphism $(\Phi^{-1}(L - L_0)u_{n_k})_k$ is convergent in $H_s^1(\mathbb{R})$, hence, $\Phi^{-1}(L-L_0)$ is a compact operator and therefore, since $\Phi^{-1}L$ is bounded, we proved the asserted compact perturbation.

Hence, since the essential spectrum is invariant under relative compact perturbations [7, Chaper IV, Theorem 5.35], the essential spectra of $\Phi^{-1}L$ and $\Phi^{-1}L_0$ coincide. Thus, we now compute the essential spectrum σ_{ess}^0 of $\Phi^{-1}L_0$.

Therefor, we consider the polynomial family

$$p_\lambda(s) := (1 - \lambda)s^2 + V - \lambda\sigma \quad \text{for all } s \in \mathbb{R}, \lambda \in \mathbb{R}.$$

We note that for all $\lambda \neq 1$ we have the following equivalence:

$$p_\lambda \text{ has real zeros} \quad \Leftrightarrow \quad \lambda \in I. \tag{17}$$

To show $\sigma_{ess}^0 \subseteq I$, let $\lambda \in \mathbb{R} \setminus I$. We will prove, that λ is in the resolvent set, i.e. for every $r \in H_s^1(\mathbb{R})$ there exists a unique $u \in H_s^1(\mathbb{R})$ such that $(\Phi^{-1}L_0 - \lambda)u = r$. Using the definition of L_0 this equality is equivalent to

$$p_\lambda(s)\mathcal{F}[u](s) = (s^2 + \sigma)\mathcal{F}[r](s) \quad \text{for all } s \in \mathbb{R}, \tag{18}$$

with $\mathcal{F}$ denoting the Fourier transform.

$\lambda \notin I$ implies that p_λ is of order 2 and has no real zeros by (17), therefore $q(s) := \frac{s^2+\sigma}{p_\lambda(s)}$ is bounded on $\mathbb{R}$ and thus, $u := \mathcal{F}^{-1}[q\mathcal{F}[r]]$ solves (18). $|\mathcal{F}[u](s)| \leq const \cdot |\mathcal{F}[r](s)|$ yields $u \in H^1(\mathbb{R})$ and, since r and q are symmetric, we get $u \in H_s^1(\mathbb{R})$ by the symmetry preserving property of $\mathcal{F}$. Furthermore, u is a unique solution of (18), since p_λ has no real zeros and thus, $r = 0$ implies $u = 0$. This proves that λ is in the resolvent set of $\Phi^{-1}L_0$ and hence not in σ_{ess}^0.

Now let $\lambda \in I \setminus \{1\}$. Due to (17) p_λ has at least one real zero s_0. We consider a function $\theta \in C^\infty(\mathbb{R})$ such that $\theta = 1$ on $(-\infty, 0]$ and $\theta = 0$ on $[1, \infty)$. Moreover, we define

$$u_n(x) := \cos(s_0 x)\theta(x - n)\theta(-x - n) \qquad \text{for all } x \in \mathbb{R}, n \in \mathbb{N}.$$

Clearly, u_n is smooth with compact support in $[-n-1, n+1]$, and $u_n(x) = \cos(s_0 x)$ on $[-n, n]$ implying

$$(L_0 u_n - \lambda\Phi u_n)(x) = [(1 - \lambda){s_0}^2 + V - \lambda\sigma]\cos(s_0 x) = p_\lambda(s_0)\cos(s_0 x) = 0$$

for all $x \in [-n, n]$. Applying Proposition 2 (b) we get

$$\|L_0 u_n - \lambda\Phi u_n\|_{H^{-1}}^2 \leq \frac{1}{\sigma}\|L_0 u_n - \lambda\Phi u_n\|_{L^2}^2 = \frac{2}{\sigma}\int_n^{n+1} |L_0 u_n - \lambda\Phi u_n|^2\, dx, \tag{19}$$

implying that $\|L_0 u_n - \lambda\Phi u_n\|_{H^{-1}}$ and thus, $\left\|\Phi^{-1}L_0 u_n - \lambda u_n\right\|_{H^1}$ is bounded as $n \to \infty$. Furthermore,

$$\|u_n\|_{H^1}^2 \geq \sigma\|u_n\|_{L^2}^2 \geq \sigma\int_{-n}^{n} \cos^2(s_0 x)\, dx \to \infty$$

as $n \to \infty$, which together with (19) yields that λ is in the spectrum of $\Phi^{-1}L_0$. We note that $\Phi^{-1}L_0$ has no eigenvalues since all solutions of $L_0u - \lambda\Phi u = 0$ are linear combinations of terms $e^{\varphi x}$ with $\varphi \in \mathbb{C}$ and thus, not in $H^1_s(\mathbb{R})$ (except 0). This yields $\lambda \in \sigma^0_{ess}$.

Finally, we prove that $\lambda = 1$ is in σ^0_{ess}. Again, $\Phi^{-1}L_0$ has no eigenvalues, wherefore it is sufficient to show that λ is in the spectrum of $\Phi^{-1}L_0$. If we suppose that λ is in the resolvent set, then $\Phi^{-1}L_0u - u = r$ would have a unique solution for all $r \in H^1_s(\mathbb{R})$, implying $r'' = \sigma r - (V - \sigma)u \in L^2_s(\mathbb{R})$ for all $r \in H^1_s(\mathbb{R})$, which obviously cannot be right. □

Isolated eigenvalues

To compute bounds for the isolated eigenvalues we first restrict the possible choices for $\sigma > 0$, i.e. we choose σ such that $\sigma > V + \frac{3}{2\sqrt{c}}\|\omega\|^2_{L^2}$. Since Γ is bounded by $\frac{1}{2\sqrt{c}}$, this choice, together with (5) and (7), yields

$$\begin{aligned}\left\langle u - \Phi^{-1}Lu, u\right\rangle_{H^1} &= (\Phi u - Lu)[u]\\ &= \int_{\mathbb{R}} \left[(\sigma - V - \Gamma * \omega^2 + 3\omega^2)u^2 - 2(\Gamma * (\omega u))\omega u\right] dx \qquad (20)\\ &\geq \int_{\mathbb{R}} \left[(\sigma - V - \frac{3}{2\sqrt{c}}\|\omega\|^2_{L^2}\right] u^2\, dx > 0\end{aligned}$$

for all $u \in H^1_s(\mathbb{R}) \setminus \{0\}$, implying the positivity of $id - \Phi^{-1}L$ on $H^1_s(\mathbb{R})$, and hence it is one-to-one. Since $\Phi^{-1}L$ is symmetric on $H^1_s(\mathbb{R})$ (see the proof of Theorem 1) and defined on the whole Hilbert space it is selfadjoint and therefore,

$$R := (id - \Phi^{-1}L)^{-1} \colon H^1_s(\mathbb{R}) \supseteq D(R) \to H^1_s(\mathbb{R}) \qquad (21)$$

is selfadjoint. Due to (20) all eigenvalues of $\Phi^{-1}L$ are less then 1 and hence, by (21), we obtain

$$\lambda \text{ is an eigenvalue of } \Phi^{-1}L \quad \Leftrightarrow \quad \frac{1}{1-\lambda} \text{ is an eigenvalue of } R. \qquad (22)$$

Moreover, the spectral mapping theorem [8, Chapter 4, Theorem 4.18] yields an analogous relation for the complete spectra, and thus especially for the essential spectrum:

$$\sigma^R_{ess} \cup \{\infty\} = \left\{\frac{1}{1-\lambda} : \lambda \in \sigma_{ess}\right\},$$

with σ^R_{ess} denoting the essential spectrum of R. Applying Proposition 2 and by the choice of σ we note that $\min \sigma_{ess} = \frac{V}{\sigma}$ and therefore, using that V and σ are positive, we deduce $\sigma_0 := \min \sigma^R_{ess} = \frac{\sigma}{\sigma - V} > 1$.

Using (21), (5) and (7) the following equivalences hold true for $\kappa \in \mathbb{R}$:

$$\begin{aligned} u \in D(R),\ Ru = \kappa u &\Leftrightarrow u \in H^1_s(\mathbb{R}),\ u = \kappa(id - \Phi^{-1}L)u\\ &\Leftrightarrow u \in H^1_s(\mathbb{R}),\ \Phi u = \kappa\Phi u - Lu\\ &\Leftrightarrow u \in H^1_s(\mathbb{R}),\ \langle u, \varphi\rangle_{H^1} = \kappa M(u, \varphi) \text{ for all } \varphi \in H^1_s(\mathbb{R}),\end{aligned}$$

with $M\colon H^1_s(\mathbb{R}) \times H^1_s(\mathbb{R}) \to \mathbb{R}$ defined by

$$M(u,\varphi) := \int_{\mathbb{R}} \left[(\sigma - V - \Gamma * \omega^2 + 3\omega^2)u\varphi - 2(\Gamma * (\omega u))\omega\varphi\right]\, dx.$$

Thus, we consider the eigenvalue problem

$$\langle u,\varphi\rangle_{H^1} = \kappa M(u,\varphi) \quad \text{for all } \varphi \in H^1_s(\mathbb{R}). \tag{23}$$

Now, we need to compute bounds for the eigenvalues neighboring 1 instead of eigenvalues neighboring 0 in the case of the eigenvalue problem for $\Phi^{-1}L$ (cf. (22)).

To calculate upper bounds the Rayleigh-Ritz method based on Poincaré's min-max principle is used (see [16, Chapter 2], [12, Theorem 40.1 and Remarks 40.1, 40.2, 39.10]):

Theorem 2 (Rayleigh-Ritz). *Let $n \in \mathbb{N}$ and $v_1,\dots,v_n \in H^1_s(\mathbb{R})$ be linearly independent. Moreover, define the matrices*

$$A_0 := \left(\langle v_i, v_j\rangle_{H^1}\right)_{i,j=1,\dots,n}, \quad A_1 := \left(M(v_i,v_j)\right)_{i,j=1,\dots,n}$$

and denote the eigenvalues of the matrix eigenvalue problem $A_0x = \hat\kappa A_1 x$ by $\hat\kappa_1 \le \dots \le \hat\kappa_n$. Then, if $\hat\kappa_n < \sigma_0$, there are at least n eigenvalues of (23) below σ_0, and the n smallest of these, ordered by magnitude and denoted by $\kappa_1,\dots,\kappa_n$, satisfy

$$\kappa_j \le \hat\kappa_j \quad (j = 1,\dots,n).$$

Lower eigenvalue bounds can be computed via the Lehmann-Goerisch Theorem (see e.g. [18, Theorem 2.4], [4, Theorem 3]), an extension of the Temple-Lehmann Theorem (see e.g. [3]), which requires as a priori information a rough lower bound for the $(n+1)$st eigenvalue if it exists below the essential spectrum. In the following we will explain how to compute such a rough bound for the $(n+1)$st eigenvalue via a homotopy method (see [4, Subsection 4.2]).

As a first step, we consider the base problem

$$\langle u,\varphi\rangle_{H^1} = \kappa^{(0)} M_0(u,\varphi) \quad \text{for all } \varphi \in H^1_s(\mathbb{R}), \tag{24}$$

with $M_0\colon H^1_s(\mathbb{R}) \times H^1_s(\mathbb{R}) \to \mathbb{R}$, $M_0(u,\varphi) := \int_{\mathbb{R}}[\sigma - V + 3\hat u^2]u\varphi\, dx$ and

$$\hat u\colon \mathbb{R} \to \mathbb{R},\ \hat u(x) := \begin{cases} \|u\|_\infty, & |x| \le R,\\ 0, & |x| > R.\end{cases}$$

Then, $M_0(u,u) \ge M(u,u)$ for all $u \in H^1_s(\mathbb{R})$ and the minimum of the essential spectrum of the base problem is again σ_0. Let $\rho_0 < \sigma_0$ be a lower bound for the essential spectrum. Since $\hat u$ is piecewise constant, we can enclose all eigenvalues of (24) below ρ_0 using fundamental solutions on $(-\infty,-R]$, $[-R,R]$ and $[R,\infty)$, respectively, and considering the corresponding matching conditions. This leads to the computation of zeros, which can be realized for example via a verified interval

Newton method or a verified bisection method (as in our case). Note that in this context it is also important to ensure that there are precisely N eigenvalues of (24) below ρ_0, i.e. we also need an index information for the N smallest eigenvalues. By the interval Newton/bisection method we indeed obtain these information.

To compare problems (23) and (24), we consider the family of bilinear forms $M_t\colon H_s^1(\mathbb{R}) \times H_s^1(\mathbb{R}) \to \mathbb{R}$ for $t \in [0,1]$ defined by

$$M_t(u,\varphi) := (1-t)M_0(u,\varphi) + tM(u,\varphi) \quad \text{for all } u,\varphi \in H_s^1(\mathbb{R})$$

and study the corresponding family of eigenvalue problems ($t \in [0,1]$)

$$\langle u,\varphi\rangle_{H^1} = \kappa^{(t)} M_t(u,\varphi) \text{ for all } \varphi \in H_s^1(\mathbb{R}). \tag{25}$$

Moreover, we note that $M_t(u,u)$ is non-increasing in t for fixed $u \in H_s^1(\mathbb{R})$. Therefore, since the essential spectra of (25) coincide for $t=0$ and $t=1$, Poincaré's min-max principle implies that the minima of the essential spectra of the eigenvalue problems (25) coincide, i.e. $\min \sigma_0^{(t)} = \sigma_0$ for all $t \in [0,1]$. Moreover, for $0 \le s \le t \le 1$ we deduce:

$$\kappa_j^{(s)} \le \kappa_j^{(t)} \text{ for all } j \text{ such that } \kappa_j^{(t)} \text{ exists below } \sigma_0,$$

with $\kappa_1^{(t)} \le \kappa_2^{(t)} \le \cdots$ denoting the eigenvalues of (25) for fixed $t \in [0,1]$.

The following Corollary ([4, Corollary 1]) is a crucial part of the homotopy which allows us to transfer the index information from (24) to (23):

Corollary 1. *Let $t \in [0,1]$ and $X := L^2(\mathbb{R}) \times L_s^2(\mathbb{R})$. Moreover, we define the bilinear form b on X by*

$$b\colon X \times X \to \mathbb{R},\ b\left(\begin{pmatrix} w_1 \\ w_2 \end{pmatrix}, \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}\right) := \langle w_1, v_1\rangle_{L^2} + \sigma \langle w_2, v_2\rangle_{L^2}.$$

Furthermore, $T\colon H_s^1(\mathbb{R}) \to X$, $Tu := (u', u)^T$ satisfies $b(Tu,Tv) = \langle u,v\rangle_{H^1}$ for all $u,v \in H_s^1(\mathbb{R})$, i.e. T is isometric. Additionally, suppose that for a given $v \in H_s^1(\mathbb{R}) \setminus \{0\}$ a $w \in X$ is in hand such that $b(w,T\varphi) = M_t(v,\varphi)$ for all $\varphi \in H_s^1(\mathbb{R})$. Finally, let $\rho \in (0,\sigma_0]$ such that there are at most finitely many eigenvalues of (25) *below ρ, and*

$$\frac{\langle v,v\rangle_{H^1}}{M_t(v,v)} < \rho.$$

Then, there is an eigenvalue κ of (25) *satisfying*

$$\frac{\rho M_t(v,v) - \langle v,v\rangle_{H^1}}{\rho b(w,w) - M_t(v,v)} \le \kappa < \rho. \tag{26}$$

Now we will give a short outline of the homotopy method (for more details see [4, Subsection 4.2]. We start with computing approximate eigenpairs $(\tilde{\kappa}_n^{(t_1)}, \tilde{u}_n^{(t_1)})$ for $n = 1,\ldots,N$ of problem (25) for some $t_1 > 0$, with $\kappa_1^{(t_1)},\ldots,\kappa_N^{(t_1)}$ ordered by magnitude. If t_1 is not too large, we may expect that the Rayleigh quotient, formed with $u_N^{(t_1)}$, satisfies $\langle u_N^{(t_1)}, u_N^{(t_1)} \rangle_{H^1} / M_{t_1}(u_N^{(t_1)}, u_N^{(t_1)}) < \rho$. Hence, Corollary 1, applied to $v = u_N^{(t_1)}$, implies the existence of an eigenvalue $\kappa^{(t_1)}$ of problem (25) (with $t = t_1$) and a lower bound ρ_1 defined by the left-hand-side of (26) such that $\rho_1 \leq \kappa^{(t_1)} < \rho$.

Successively, we can continue this procedure with $t_2 > t_1$ etc. until either $t_N < 1$ (i.e. the homotopy cannot be continued) or $t_r = 1$ for some $1 \leq r \leq N$ which is the case in all our examples. Thus, problem (25) with $t = t_r = 1$ has at most $N - r$ eigenvalues below ρ_r. Using a Rayleigh-Ritz computation, we can finally check that there are at least $N - r$ eigenvalues below ρ_r and hence, there are precisely $N - r$ eigenvalues in $(0, \rho_r)$. In all our examples only one eigenvalue remained after the homotopy (i.e. $N - r = 1$), hence, there is no need for an additional Lehmann-Goerisch computation and we can compute the desired eigenvalue bound directly from the Rayleigh-Ritz computation and the homotopy bound ρ_r (see Figure 2).

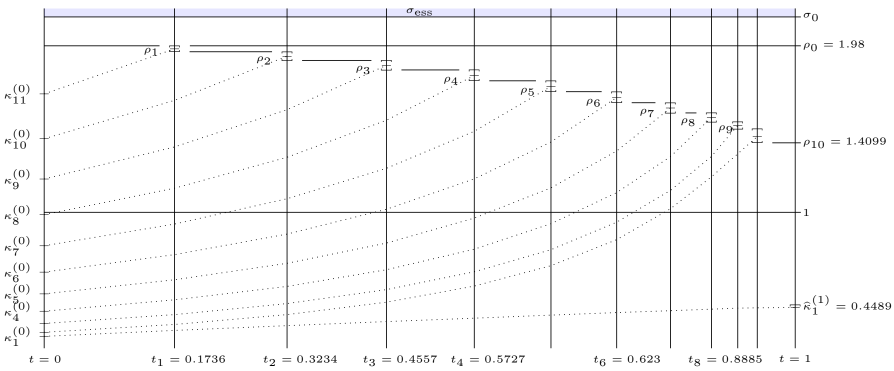

Figure 2: Course of the homotopy for $c = 50$

3 Numerical Results

In this section we will give a short overview about our numerical results with the specific potential $V = 1.0$. Using the Newton steps described in Subsection 2.1 we compute approximate solutions to the one-dimensional Schrödinger-Poisson system (2) for different values of c (see Figure 3). For the computation we set R to 10.0 and use between 40 and 50 ansatz functions varying with the value of c. In all cases the parameter p, used in the Newton methods introduced in Subsection 2.1, passes the values $0, 0.5, 1$ and the defect bound δ computed via the techniques decribed in Subsection 2.2 is of order 10^{-4}.

Using the methods stated in Subsection 2.3 we are able to calculate upper bounds for the eigenvalues "nearby" 1 in all considered cases. However, the homotopy algorithm und thus the computation of lower bounds failed in cases where

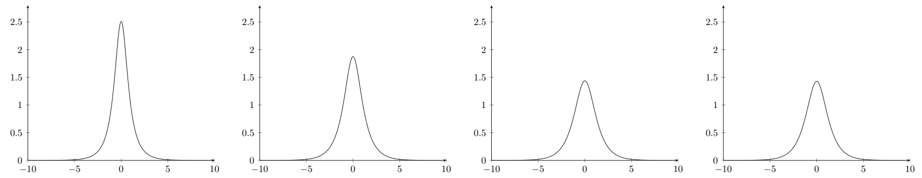

Figure 3: Approximate solutions for $c = 1.0,\ 2.0,\ 30.0,\ 50.0$ (from left to right)

c is smaller than 30. In the remaining situations we can compute constants K satisfying (10). Applying Theorem 1 to these approximate solutions we are able to prove existence of a non-trivial solution (see Table 1).

Table 1: Numerical results in the successful cases

c	V	σ	δ	σ_0	ρ_0	K	α
30.0	1.0	2.133	3.085e-4	≈ 1.8826	1.88	3.753	1.17e-3
40.0	1.0	1.973	3.154e-4	≈ 2.0277	2.02	3.543	1.12e-3
50.0	1.0	1.866	3.174e-4	≈ 2.1547	1.98	3.498	1.12e-3

4 Concluding Remarks and Outlook

Concerning the potential, Theorem 1 can easily be generalized, i.e. we can replace the constant potential V by a symmetric positive potential in $L^\infty(\mathbb{R})$ satisfying $\lim_{x\to\infty} V(x) = \lim_{x\to-\infty} V(x) > 0$. Additionally, the non-linearity can be replaced by a more general function $f \in C^1(\mathbb{R})$. In this generalized setting Theorem 1 remains valid, however, the proof has to be adapted at some stages. Although, the computation of approximate solutions is a more difficult task since it is a priori unknown how to start the Newton iteration (cf. Subsection 2.1).

As written in the beginning, the considered one-dimensional system only provides as a basis for the three-dimensional stationary version (1). The applicability of computer-assisted methods in three-dimensional case still remains an open question. Furthermore, the time-dependent Schrödinger-Poisson system remains a task for future research.

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