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Pseudomodes of Schrödinger operators

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Pseudomodes of non-self-adjoint Schrödinger operators corresponding to large pseudoeigenvalues are constructed. The approach is non-semiclassical and extendable to other types of models including the damped wave equation and Dirac operators.

KEYWORDS
pseudospectrum, non-self-adjointness, Schrödinger operators, complex potentials, WKB method

1 Introduction

The (ε-)pseudospectrum $\sigma_\varepsilon(H)$ (with positive ε) of an operator H in a Hilbert space is the union of the spectrum $\sigma(H)$ of H and all those complex numbers λ from the resolvent set $\rho(H)$ of H for which

$$\|(H-\lambda)^{-1}\| > \frac{1}{\varepsilon}.$$

Equivalently, $\sigma_\varepsilon(H)$ comprises the spectrum of H and $\lambda \in \mathbb{C}$ (pseudoeigenvalues) for which there exists a vector ψ (pseudomode) in the domain of H such that

$$\|(H-\lambda)\psi\| < \varepsilon\|\psi\|.$$

If H is self-adjoint (or, more generally, normal), the ε-pseudospectrum is trivial in the sense that it is just the ε-tubular neighbourhood of the spectrum of H. In general, however, the pseudoeigenvalues can lie outside the ε-tubular neighbourhood and their location is important to correctly seize various properties of H, see [1–3].

The goal of this brief research report is to explain in a succinct way the approach in Krejčiřík and Siegl [4] to locate pseudoeigenvalues of (non-semiclassical) Schrödinger operators

$$-\frac{d^2}{dx^2} + V(x) \qquad \text{in} \qquad L^2(\mathbb{R}), \tag{1}$$

where $V: \mathbb{R} \to \mathbb{C}$ is at least locally square-integrable and $\Re V \geq 0$. In such a case, there exists a unique m-accretive extension H_V of Equation 1 initially defined on $C_0^\infty(\mathbb{R})$, see ([5], Thm. VII.2.6). Since our constructed pseudomodes are compactly supported and at least twice weakly differentiable, they belong to the domain of H_V.

The operator H_V is self-adjoint (respectively, normal) if, and only if, V is real-valued (respectively, $\Im V$ is constant). To ensure non-trivial pseudospectra, we shall therefore adopt the standing hypothesis

$$\limsup_{x\to-\infty} \Im V(x) < 0 < \liminf_{x\to+\infty} \Im V(x), \tag{2}$$

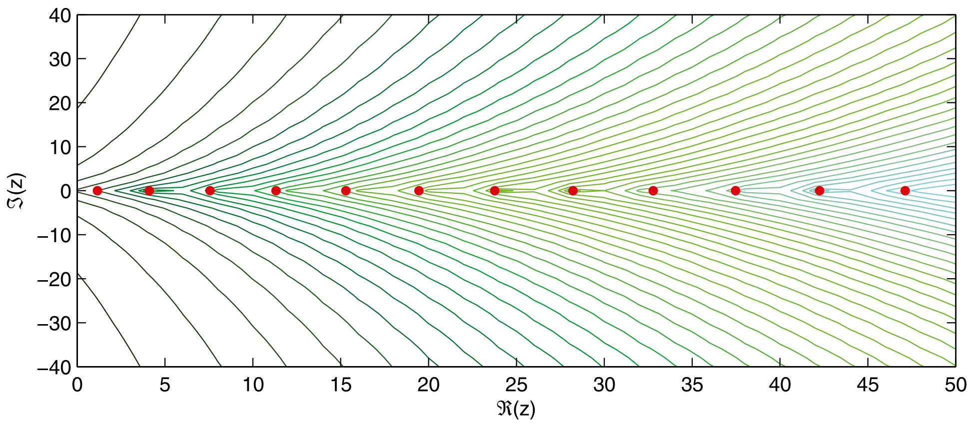

FIGURE 1
Spectrum (red dots) and pseudospectra (enclosed by the green contour lines) of the imaginary cubic oscillator. (Courtesy of Miloš Tater.)

where the limits are allowed to be infinite. The assumption (Equation 2) can be interpreted as a "global" version of the Davies' condition $\Im V' \neq 0$, see [6] and also [7].

To simplify the presentation, the potential V will be assumed to be smooth and imaginary-valued. Typical examples to keep in mind are as follows:

$$V_1(x) := i\arctan(x), \qquad V_2(x) := ix^m \quad \text{with} \quad m\,\text{odd}, \\ V_3(x) := i\sinh(x), \tag{3}$$

or their imaginary shifts. In particular, V_2 with $m = 3$ is the celebrated imaginary cubic (or Bender's) oscillator (with purely real and discrete spectrum, see Figure 1), which was made popular in the context of the so-called $\mathcal{PT}$-symmetric quantum mechanics in [8].

The objective is to develop a systematic construction of pseudomodes ensuring that, for any diminishing $\varepsilon \to 0$, there is a complex number λ with large magnitude $|\lambda| \to \infty$ such that $\lambda \in \sigma_\varepsilon(H_V)$. The results are particularly striking whenever this set of pseudoeigenvalues lie outside (in fact, "very far" from) the ε-tubular neighbourhood of $\sigma(H)$. This is particularly the case of the imaginary cubic oscillator, for which the analysis below show that for an arbitrarily small ε there exists a pseudoeigenvalue λ with an arbitrarily large imaginary part, despite the fact that the spectrum is purely real (see Figure 1 for a numerical quantification of the pseudospectrum level lines). This property implies the lack of Riesz basis for the eigenfunctions, challenging in the spirit of [9] the physical relevance of the $L^2(\mathbb{R})$-realisation of the Bender's oscillator. The follow-up [4] summarised in this report can be considered as a methodical and more advanced study of not necessarily polynomial potentials.

The feature of the approach of [4] is that it does not rely on semiclassical methods developed in [6, 7, 10]. In fact, we are able to construct large-energy pseudomodes for potentials (like of exponential type, see V_3 of Equation 3) which cannot be reduced (by scaling) to a small Planck's constant included in the kinetic energy. On the contrary, the known claims in the semiclassical setting follow immediately from our approach.

2 Methods

Our strategy of the construction of pseudomodes is based on the Liouville–Green approximation, also known as the JWKB method in mathematical physics. The key idea is that, if V were constant, exact solutions of the differential equation associated with $H_V g = \lambda g$ would be the two non-integrable functions

$$g_\pm(x) := \exp\left(\pm i \int_0^x \sqrt{\lambda - V(t)}\,\mathrm{d}t\right).$$

The starting point of the approximation scheme is to use the same ansatz for variable V as well. More specifically, we choose $g_0 := g_-$ for it is exponentially decaying under the hypothesis (Equation 2), whenever $\Im\lambda$ is small with respect to the limits of $\Im V$ at $\pm\infty$. A direct computation yields

$$(H_V - \lambda)g_0 = r_0\, g_0 \qquad \text{with} \qquad r_0 := -\frac{i}{2}\frac{V'}{\sqrt{\lambda - V}}. \tag{4}$$

Recalling the simplifying hypothesis that $\Re V = 0$ and assuming in addition that $\Im\lambda = 0$ and $\Re\lambda > 0$ (typically large), one has the estimate

$$\|r_0\|_\infty \leq \frac{1}{\sqrt{\Re\lambda}^{\,1-\delta}} \left\| \frac{|V'|}{2|V|^{\delta/2}} \right\|_\infty \tag{5}$$

for every $\delta \in [0, 1)$. It follows that large real energies always lie in the pseudospectrum, namely, for every positive ε,

$$\left\{ \lambda \in \mathbb{C}: \ \sqrt{\Re\lambda}^{\,1-\delta} > \frac{1}{\varepsilon} \left\| \frac{|V'|}{2|V|^{\delta/2}} \right\|_\infty \right\} \subset \sigma_\varepsilon(H_V).$$

Of course, this result is interesting only if the supremum norm is bounded. From examples (Equation 3), relevant potentials are thus V_1 and V_2 with $m = 1$, in which case we can take $\delta = 0$ and obtain thus a pseudomode satisfying the decay $\|(H_V - \lambda)g_0\| = O((\Re\lambda)^{-1/2})\,\|g_0\|$ as $\Re\lambda \to \infty$. The latter is particularly interesting because the spectrum of the imaginary Airy operator is empty, see, e.g., ([3, 11], Section VII.A) or more generally [12], where the last reference includes also an elementary proof of the optimal resolvent norm estimate for the Airy operator.

It is not difficult to modify the exponentially decaying pseudomode g_0 to a compactly supported pseudomode f_0, while still keeping the same decay $\|(H_V-\lambda)f_0\| = O((\Re\lambda)^{-1/2})\|f_0\|$ as $\Re\lambda \to \infty$. Indeed, let $\xi_1 : \mathbb{R} \to [0,1]$ be a smooth function such that $\xi_1 = 1$ on $[-1,1]$ and $\xi_1 = 0$ outside $[-2,2]$. Given any positive number l, let us define the rescaled cut-off function $\xi_l(x) := \xi_1(x/l)$. Then $f_0 := \xi_l g_0$ is compactly supported and one has

$$(H_V-\lambda)f_0 = \xi_l H_V g_0 + \left(-\xi_l'' + 2i\sqrt{\lambda - V}\,\xi_l'\right)g_0.$$

Using that $\xi_l \to 1$ pointwise as $l \to \infty$, while one gains one l^{-1} by each derivative, it is possible to verify the desired decay by the λ-dependent choice $l := \Re\lambda$.

To cover a larger class of potentials, let us consider a modified ansatz $g_1 := g_0 \exp(-\psi_0)$, where ψ_0 is a function to be chosen later. A direct computation yields

$$(H_V-\lambda)g_1 = \left(r_0 - 2i\sqrt{\lambda - V}\,\psi_0' + \psi_0'' - \psi_0'^2\right)g_1.$$

Now we choose ψ_0 to annihilate the error term r_0 from Equation 4, by solving the first-order linear differential equation $r_0 - 2i\sqrt{\lambda - V}\psi_0' = 0$, namely, $\psi_0 := \log\sqrt[4]{\lambda - V}$. Thus we arrive at the familiar expression

$$g_1(x) = \frac{1}{\sqrt[4]{\lambda - V(x)}}\exp\left(-i\int_0^x \sqrt{\lambda - V(t)}\,\mathrm{d}t\right).$$

Then

$$(H_V-\lambda)g_1 = r_1 g_1 \qquad \text{with} \qquad r_1 := -\frac{5}{16}\frac{V'^2}{(\lambda - V)^2} - \frac{1}{4}\frac{V''}{\lambda - V},$$

where the new error term r_1 can be estimated as follows:

$$\|r_1\|_\infty \le \frac{1}{\sqrt{\Re\lambda}^{2(1-\delta)}}\left\|\frac{5|V'|^2}{16|V|^{1+\delta}} + \frac{|V''|}{4|V|^\delta}\right\|_\infty.$$

This result is an improvement upon (Equation 4) with (Equation 5) in two respects. First, if the supremum norm is bounded for $\delta = 0$, we get a pseudomode with an improved decay $\|(H_V-\lambda)g_1\| = O((\Re\lambda)^{-1})\|g_1\|$ as $\Re\lambda \to \infty$. This is the case of V_1 and V_2 with $m = 1$ from examples (Equation 3). Second, keeping the decay $O((\Re\lambda)^{-1/2})$ by the choice $\delta = 1/2$, we can now cover V_2 with $m = 3$ from examples (Equation 3).

The above scheme can be continued by employing the general ansatz in square-root powers of λ:

$$g_k = \exp\left(-\lambda^{1/2}\psi_{-1} + \lambda^{-0/2}\psi_0 + \lambda^{-1/2}\psi_1 + \cdots + \lambda^{-(k-1)/2}\psi_{k-1}\right), \quad (6)$$

where $\psi_{-1}(x) := i\lambda^{-1/2}\int_0^x \sqrt{\lambda - V(t)}\,\mathrm{d}t$ and ψ_{k-1} with $k \in \mathbb{N}$ is iteratively chosen in such a way to annihilate the previous error term r_{k-1}. By enlarging k, more derivatives of V are required. On the other hand, a better decay (in negative powers of $\Re\lambda \to \infty$) of the new error term is achieved and a larger class of potentials can be covered. For instance, all the examples (Equation 3) are already covered by the choice $k = 2$, namely, $\|(H_V-\lambda)g_2\| = O((\Re\lambda)^{-1/2})\|g_2\|$ as $\Re\lambda \to \infty$.

3 Results

To make the above procedure rigorous, it is important to ensure that g_0 in the expansion (Equation 6) is dominant, in order to guarantee that $g_k(x)$ have appropriate decay properties at $x = \pm\infty$. One of the main achievements of [4] is the formulation of the robust sufficient condition

$$\frac{|V^{(n)}(x)|}{|V(x)|} = O(|x|^{n\nu}) \qquad \text{and} \qquad |x|^{4(1+\nu)} = O(|V(x)|) \quad (7)$$

to hold as $|x| \to \infty$ with some real number $\nu \le 0$ for every $n = 1, \ldots, k+1$. Note that $\nu = -2, -1$ and 0 for the potentials V_1, V_2 and V_3 of Equation 3, respectively. In fact, it is possible to allow for $\nu > 0$ (corresponding to superexponentially growing potentials). Moreover, different behaviours at $x \to \pm\infty$ may be allowed. However, let us stick to Equation 7 to make the presentation here as simple as possible.

To get a compactly supported pseudomode, it turns out that the adequate λ-dependent cut-off function should be supported in the interval $[-l_-, l_+]$, where (denoting $\langle l\rangle := (1 + l^2)^{1/2}$)

$$l_\pm := \begin{cases} \inf\left\{l \ge 0 : \dfrac{|V(\pm l)|^2}{\langle l\rangle^{4(1+\nu)}} = \lambda\right\} & \text{if } V \text{ is unbounded at } \pm\infty, \\ \lambda^{1-\frac{\nu}{4}} & \text{if } V \text{ is bounded at } \pm\infty. \end{cases}$$

Recall that we assume $\Im\lambda = 0$ and note that $l_\pm \to \infty$ as $\lambda \to \infty$. In particular, $l_\pm = \lambda^{3/2}, \lambda^{1/(2m)}$ and $\log\lambda$ as $\lambda \to \infty$ for the potentials V_1, V_2 and V_3 of Equation 3, respectively.

Under the present simplifying hypotheses (in particular, $\Im\lambda = 0$, $\Re V = 0$ and $\nu \le 0$), the general result of Krejčiřík and Siegl [4] (Thm. 3.7) can be formulated as follows.

Theorem 1. Let $V : \mathbb{R} \to i\mathbb{R}$ be smooth satisfying Equations 2, 7 with given $k \in \mathbb{N}$. If

$$\lambda^{-(k+1)/2} \sup_{x\in(-l_-, l_+)} |V(x)|\,\langle x\rangle^{(k+1)\nu} \xrightarrow[\lambda\to+\infty]{} 0, \quad (8)$$

then there exists $\{\psi_\lambda\}_\lambda \subset C_0^\infty(\mathbb{R})$ such that $\|\psi_\lambda\| = 1$ and

$$\lim_{\lambda\to+\infty}\|(H_V-\lambda)\psi_\lambda\| = 0. \quad (9)$$

The extra condition (Equation 8) with the choice $k = 0$ is clearly satisfied for the potential V_1 of Equation 3 (in fact, for any bounded potential satisfying Equations 2, 7). To satisfy Equation 8 for all the polynomial potentials V_2 of Equation 3, it is sufficient to take $k = 1$. Finally, Equation 8 is verified for the exponential potential V_3 of Equation 3 with $k = 2$.

In Krejčiřík and Siegl [4], the decay rate in Equation 9 is carefully quantified in terms of the left-hand side of Equation 8 and other quantities related to the behaviour of a general potential V at infinity.

4 Discussion

4.1 Generality

The JWKB-type scheme sketched in Section 2 is made rigorous in [4] for a fairly general class of potentials V, beyond the present simplifying hypotheses. In particular, the potential V is allowed to have a real part, however, its largeness must be suitably “small” with respect to its imaginary part. This is quantified by natural modifications of Equations 2, 7. What is more, pseudoeigenvalues along general curves (beyond the present simplifying hypothesis $\Im\lambda = 0$) diverging in the complex plane are located. In particular, the rotated harmonic (or Davies') oscillator $V(x) = ix^2$ made popular in the pioneering work [13] or shifted harmonic oscillator $V(x) = (x+i)^2$ studied in [3, 14] are covered. At the same time, potentials decaying at infinity are included. Finally, possibly discontinuous potentials (like $V(x) = i\,\mathrm{sgn}(x)$) are comprised by a refined mollification argument.

4.2 Optimality

It turns out that the conditions on potentials identified in [4] as well as the regions in the complex plane where the pseudoeigenvalues are located are optimal. The latter can be checked directly for the rotated harmonic (or Davies') oscillator $V(x) = ix^2$ with help of the conjecture due to [15] solved by [16], More generally, the optimality of the pseudospectral regions follows by upper resolvent estimates performed in [17, 18].

4.3 Generalisations

The method of [4] is fairly robust and can be generalised to other models. So far, this has been done for the damped wave equation in [19], Dirac operators in [20] and biharmonic operators in [21].

Data availability statement

The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding author.

Author contributions

DK: Writing–review and editing, Writing–original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal Analysis, Data curation, Conceptualization. PS: Writing–review and editing, Writing–original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal Analysis, Data curation, Conceptualization.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

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