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Proc. R. Soc. Lond. A 1999 **455**, 585-599
doi: 10.1098/rspa.1999.0325

THE ROYAL SOCIETY

Pseudo-spectra, the harmonic oscillator and complex resonances

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Received 3 February 1998; accepted 1 May 1998

We prove that non-self-adjoint harmonic and anharmonic oscillator operators have non-trivial pseudo-spectra. As a consequence, the computation of high-energy resonances by the dilation analyticity technique is not numerically stable.

Keywords: harmonic oscillator; anharmonic oscillator; complex resonances; pseudo-spectrum; dilation analyticity; resolvent norms; JWKB method

1. Introduction

In a series of recent papers Trefethen and others have shown that the spectra of non-self-adjoint linear operators can be highly unstable under small perturbations, and have introduced the notion of pseudo-spectra that provide information about the extent of this instability (Böttcher 1994, 1995; Davies 1997; Reddy 1993; Reddy & Trefethen 1994; Reichel & Trefethen 1992; Trefethen 1992, 1997). In this paper we apply these ideas to some typical quantum-mechanical Hamiltonians, and discover that their spectra are both numerically and theoretically unstable under analytic continuation. Our theorems concern the high-energy asymptotic instability of eigenvalues/complex resonances, while the numerical results show that these instabilities develop at remarkably low energies.

We start by investigating the simplest case, that of the harmonic oscillator, for which the calculations are particularly simple, but apparently new. We then consider certain anharmonic oscillators and also a self-adjoint quantum-mechanical Hamiltonian that has complex resonances located near a reflecting barrier. We show that the use of the standard technique of dilation analyticity for this operator leads to intrinsic instabilities in locating high-energy resonances, by virtue of the same pseudo-spectral behaviour, as occurs for many other non-self-adjoint operators.

Sections 2 and 3 of this paper concern the operator

$$Hf(x) = -\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + cx^2 f(x)$$

acting on $L^2(\mathbb{R})$, where c is a complex constant satisfying $\mathrm{Re}(c) > 0$ and $\mathrm{Im}(c) > 0$. This operator has a closed sectorial form with form domain independent of c, and the resolvent operators $(H - zI)^{-1}$ are compact for all z not in the spectrum $\mathrm{spec}(H)$ of H (Kato 1966). Since the eigenvalues of H may be written down in closed form for positive real c, an analytic continuation argument proves that the spectrum of H must be

$$\{c^{1/2}(2n-1) : n = 1, 2, \dots\}.$$

In theorem 2.6 we prove that the eigenfunctions of H do not form an unconditional basis of the Hilbert space. Second, H is not similar to a normal operator, that is there does not exist any bounded invertible operator S such that SHS^{-1} is normal. Indeed there does not exist any constant a such that

$$\|(H - zI)^{-1}\| \leqslant a \operatorname{dist}(z, \operatorname{spec}(H))^{-1}$$

for all $z \notin \operatorname{spec}(H)$. We actually prove much more, namely

$$\lim_{r \to +\infty} \|(H - r\mathrm{e}^{\mathrm{i}\theta} I)^{-1}\| = +\infty$$

for all θ satisfying $0 < \theta < \arg(c)$; see theorem 2.5. In theorem 2.7 we show that these statements do not depend upon the exact potential chosen. They are stable under perturbations by bounded potentials that vanish at infinity. In other words they depend only upon the asymptotic form of the potential.

The results can be interpreted in the language of pseudo-spectral theory. If we define $\operatorname{spec}_\varepsilon(H)$ for any $\varepsilon > 0$ to be the union of $\operatorname{spec}(H)$ with the set of all z such that $\|(H - zI)^{-1}\| > \varepsilon^{-1}$, then $\operatorname{spec}_\varepsilon(H)$ contains the ε-neighbourhood of $\operatorname{spec}(H)$, but may be much larger. The size of these pseudo-spectral regions provides a clear indication of the instability of $\operatorname{spec}(H)$ under small perturbations by virtue of the formula

$$\operatorname{spec}_\varepsilon(H) = \cup\{\operatorname{spec}(H + A) : \|A\| < \varepsilon\}. \tag{1.1}$$

See the references above for proofs of these and related statements about pseudo-spectra.

Section 4 treats the same problem for a Schrödinger operator acting on $L^2(\mathbb{R})$ whose potential V is asymptotically given by a complex multiple of a positive power of the space variable x as $x \to +\infty$, culminating in corollary 4.5. This allows us in § 5 to discuss the resonances of a semi-bounded self-adjoint Schrödinger operator for which $V(x) \to 0$ as $x \to -\infty$ and $V(x) - x \to 0$ as $x \to +\infty$. We show that the determination of the resonances of this operator using the method of dilation analyticity needs to be treated with caution. The spectrum of the analytically continued operator is intrinsically unstable far from the origin, so numerical approaches to its computation are fraught with difficulties. Numerical studies in § 5 show that the onset of these problems is remarkably quick.

It is quite possible that our main results could be proved by a careful analysis of the Green function, but we actually exhibit the pseudo-eigenfunctions explicitly, since we consider that this has independent interest and is more adaptable to related problems in higher dimensions.

2. The harmonic oscillator

We construct a function f_η on $\mathbb{R}$ parametrized by the positive real number η. Throughout the section the term 'constant' refers to quantities that may depend on c and another number $\alpha > 0$, but not on η, which will be allowed to diverge to $+\infty$ at the end of the argument. We will see that the function f_η is concentrated around the point $x_0 := \alpha\eta > 0$. The function f_η is a smooth truncation of the JWKB-type function

$$\phi(x) := \mathrm{e}^{-\psi(x)},$$

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where

$$\psi(x_0+s) := \psi_1 s + \tfrac{1}{2}\psi_2 s^2 + \tfrac{1}{3}\psi_3 s^3$$

for all $s \in \mathbb{R}$. Note that ϕ is not Gaussian and does not lie in L^2. Motivated by the JWKB analysis we put

$$\begin{aligned}\psi_1 &:= \mathrm{i}\eta,\\ \psi_2 &:= -\mathrm{i}c\alpha,\\ \psi_3 &:= \gamma/\eta,\end{aligned}$$

where

$$\gamma := -\tfrac{1}{2}\mathrm{i}(c^2\alpha^2 + c).$$

A direct computation establishes first that

$$(H\phi)/\phi = \psi'' - (\psi')^2 + cx^2,$$

and then that

$$H\phi(x_0+s) = (p(s)+z)\phi(x_0+s),$$

where

$$\begin{aligned}p(s) &:= 2\gamma s/\eta + 2\mathrm{i}c\alpha\gamma s^3/\eta - \gamma^2 s^4/\eta^2\\ z &:= \eta^2 + c\alpha^2\eta^2 - \mathrm{i}c\alpha.\end{aligned}$$

Lemma 2.1. *There exist positive constants β_2 and β_3 such that*

$$|\phi(x_0+s)|^2 = \exp[-\beta_2 s^2 - \beta_3 s^3/\eta]$$

for all $s \in \mathbb{R}$. The left-hand side has a local maximum at $s = 0$ and a local minimum at

$$s_0 := -\tfrac{2}{3}\beta_2\eta/\beta_3 < 0.$$

Proof. Putting $c := c_1 + \mathrm{i}c_2$, a direct calculation shows that

$$\begin{aligned}\beta_2 &:= c_2\alpha,\\ \beta_3 &:= \tfrac{1}{3}c_2(2c_1\alpha^2 + 1),\end{aligned}$$

both of which are evidently positive.

We truncate ϕ to the left of its local maximum as follows. It is routine to construct a C^∞ function $g : \mathbb{R} \to [0,1]$ with the following properties for suitable constants β_i. We require $g(s) = 0$ for $s \leqslant s_0$, $g(s) = 1$ for $s \geqslant \frac{1}{2}s_0$, $|g'(s)| \leqslant \beta_4/|s_0|$ for $s_0 \leqslant s \leqslant \frac{1}{2}s_0$ and $|g''(s)| \leqslant \beta_5/|s_0|^2$ for $s_0 \leqslant s \leqslant \frac{1}{2}s_0$. Given such a function we now define

$$f_\eta(x_0+s) := \phi(x_0+s)g(s)$$

for all $s \in \mathbb{R}$. It is clear that

$$f_\eta \in \mathrm{dom}(H) \subset L^2(\mathbb{R}).$$

■

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Lemma 2.2. *The function f_η has the following properties:*

$$
\begin{aligned}
\mathrm{e}^{-2\beta_2 s^2} \leqslant |f_\eta(x_0+s)|^2 &\leqslant \mathrm{e}^{-\beta_2 s^2}, && \text{if } 0 \leqslant s \leqslant |s_0|,\\
\mathrm{e}^{-\beta_2 s^2} \leqslant |f_\eta(x_0+s)|^2 &\leqslant \mathrm{e}^{-\beta_2 s^2/3}, && \text{if } \tfrac{1}{2}s_0 \leqslant s \leqslant 0,\\
|f_\eta(x_0+s)|^2 &\leqslant \mathrm{e}^{-\beta_2 s^2}, && \text{if } s \geqslant |s_0|,\\
|f_\eta(x_0+s)|^2 &\leqslant \mathrm{e}^{-\beta_2 s^2/3}, && \text{if } s_0 \leqslant s \leqslant \tfrac{1}{2}s_0,\\
f_\eta(x_0+s) &= 0, && \text{if } s \leqslant s_0.
\end{aligned}
$$

The proof follows immediately from the formula

$$|f_\eta(x_0+s)|^2 = g(s)^2 \exp\left[-\beta_2 s^2\left(1-\frac{2s}{3s_0}\right)\right],$$

as do the statements of the following lemma.

Lemma 2.3. *There exist constants β_6 and β_7 such that*

$$
\begin{aligned}
|g'(s)\phi'(x_0+s)|^2 &\leqslant \beta_6 \mathrm{e}^{-\beta_2 s^2/3},\\
|g''(s)\phi(x_0+s)|^2 &\leqslant \beta_7 \eta^{-4} \mathrm{e}^{-\beta_2 s^2/3},
\end{aligned}
$$

for all $s_0 \leqslant s \leqslant \frac{1}{2}s_0$, the left-hand sides vanishing for all other s.

We can now prove the main theorem of the section, which states that H has a continuum of pseudo-eigenfunctions (parametrized by α and η), which are not closely related to its true eigenfunctions.

Theorem 2.4. *The functions f_η satisfy*

$$\lim_{\eta\to+\infty} \|Hf_\eta - z_\eta f_\eta\|/\|f_\eta\| = 0,$$

where

$$z_\eta := \eta^2 + c\alpha^2\eta^2 - \mathrm{i}c\alpha.$$

Hence

$$\lim_{\eta\to+\infty} \|(H - z_\eta I)^{-1}\| = +\infty.$$

Proof. We have

$$Hf_\eta(x_0+s) = g(s)H\phi(x_0+s) - 2g'(s)\phi'(x_0+s) - g''(s)\phi(x_0+s).$$

By applying the formulae already proved we get

$$Hf_\eta(x_0+s) - z_\eta f_\eta(x_0+s) = p(s)\phi(x_0+s) - 2g'(s)\phi'(x_0+s) - g''(s)\phi(x_0+s).$$

The estimates of lemmas 2.2 and 2.3 now enable us to complete the proof without trouble. ∎

Theorem 2.4 leads quickly to various other statements, which appear to be new.

Theorem 2.5. *If $0 < \theta < \arg(c)$, then*

$$\lim_{r\to+\infty} \|(H - r\mathrm{e}^{\mathrm{i}\theta} I)^{-1}\| = +\infty.$$

If, however, $\arg(c) < \theta < 2\pi$, then

$$\lim_{r\to+\infty} \|(H - r\mathrm{e}^{\mathrm{i}\theta} I)^{-1}\| = 0.$$

Proof. The first statement depends upon the observation that by choosing $\alpha > 0$ appropriately, the limit of $\arg(z_\eta)$ as $\eta \to +\infty$ can take any value in $(0, \arg(c))$, together with a local uniformity argument with respect to α. We next observe that the numerical range of H lies in $N := \{z : 0 \leqslant \arg(z) \leqslant \arg(c)\}$. A general argument (Davies 1997) now implies that

$$\|(H - zI)^{-1}\| \leqslant \operatorname{dist}(z, N)^{-1}$$

for all $z \notin N$, which implies the second statement. ∎

Theorem 2.6. *There does not exist a bounded invertible operator S on $L^2(\mathbb{R})$ such that SHS^{-1} is normal. Moreover, the set of eigenfunctions of H does not form an unconditional or Riesz basis.*

Proof. If such an operator S existed, then we could deduce the estimate

$$\|(H - zI)^{-1}\| \leqslant \|S\|\,\|S^{-1}\|\operatorname{dist}(z, \operatorname{spec}(H))^{-1},$$

which contradicts the resolvent bounds proved above. If the set $\{\phi_n\}$ of normalized eigenfunctions of H were an unconditional basis, then there would exist a bounded invertible operator S such that $\{S\phi_n\}$ is a complete orthonormal set in $L^2(\mathbb{R})$ (Gohberg & Krein 1969). It would follow that SHS^{-1} is a normal operator. ∎

The results obtained above do not depend on having a quadratic potential: only the asymptotic form of the potential is important.

Theorem 2.7. *Let K be the non-self-adjoint operator*

$$Kf(x) = -\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + cx^2 f(x) + V(x)f(x)$$

on $L^2(\mathbb{R})$, where $\operatorname{Re}(c) > 0$, $\operatorname{Im}(c) > 0$ and V is a bounded complex potential such that $\lim_{|x|\to\infty} V(x) = 0$. Then the conclusions of theorems 2.4, 2.5 and 2.6 are still valid with K replacing H.

Proof. The only point that needs attention is that one must ensure that the pseudo-eigenfunctions f_η have supports that tend to infinity as $\eta \to +\infty$, so that the influence of the perturbing potential vanishes in this limit. This is achieved by adopting the new definition $s_0 := -\frac{1}{2}\alpha\eta$ in lemma 2.1. ∎

3. Numerical results

We illustrate the theoretical results with the numerical computations that led us to them in the first place. The results suggest that the rate of divergence of the resolvent norm along rays is exponential, which is far more than we have proved. It is not our goal to obtain precise numerical results for the operator discussed theoretically above, but rather to show the phenomena already described using a simple discretization of the problem. A more accurate numerical simulation of the differential operator by Trefethen, based upon Chebyshev spectral collocation rather then finite differences, has confirmed the results described below (L. N. Trefethen, personal communication).

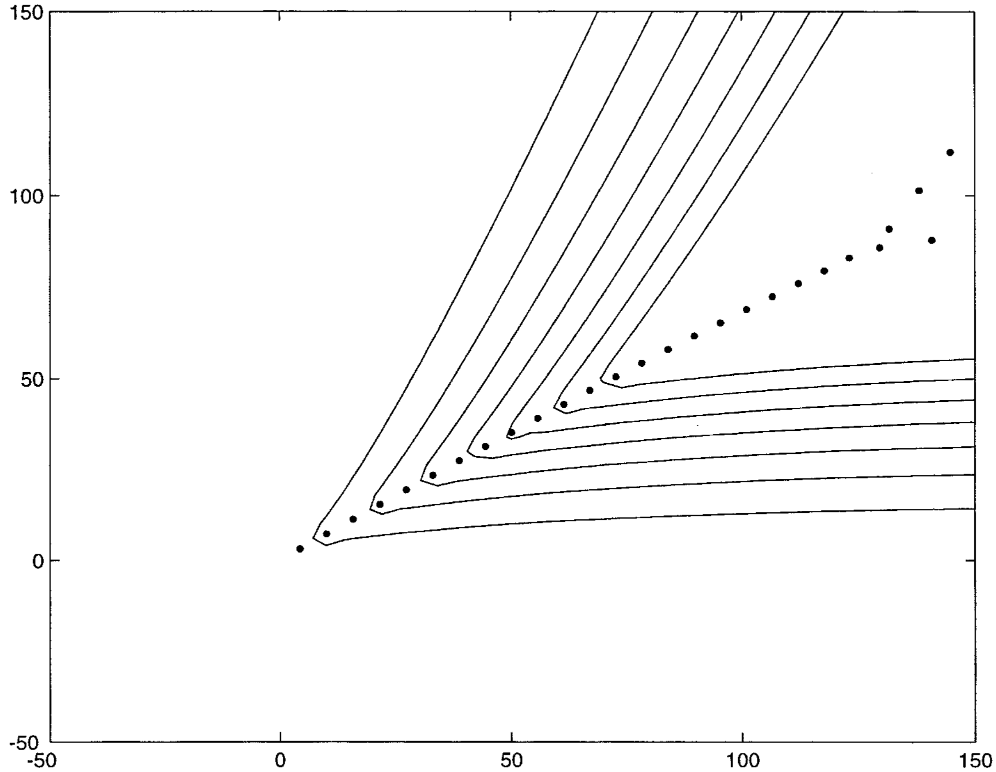

Figure 1. Harmonic oscillator eigenvalues and pseudo-spectra.

The operator H is invariant with respect to reflection about the origin, and we only examine the odd subspace. More precisely, we look at the associated difference operator on $l^2\{1,\dots,N\}$, where $N = mb$, b is the length of the interval and m is the number of points uniformly distributed in any unit interval. We repeated the calculations for a range of values of b and m to check the reliability of the results. Of course, since the computations confirm the results that we have already proved, this is not really necessary! We then replace the operator H by the associated matrix A defined by

$$A_{r,s} := \begin{cases} -m^2, & \text{if } |r-s| = 1, \\ c(r/m)^2 + 2m^2, & \text{if } r = s, \\ 0, & \text{otherwise.} \end{cases}$$

All of our calculations have been carried out with the particular choice $c = 1 + 3\mathrm{i}$. We found that with $b = 16$ and $m = 20$ the 20 eigenvalues of A closest to the origin are within 1% of the theoretically predicted values, and thus lie close to the line

$$\{z : \arg(z) = \tfrac{1}{2}\arg(c)\}.$$

We used MATLAB to calculate the singular values of $H - zI$ for $b = 16$ and $m = 10$ and a range of values of z, and then plotted level curves of the results in figure 1. The method of computation is discussed in § 5. The level curves correspond to values of the resolvent norm ranging from 1 for the outside contour in multiples of 10 to 10^6

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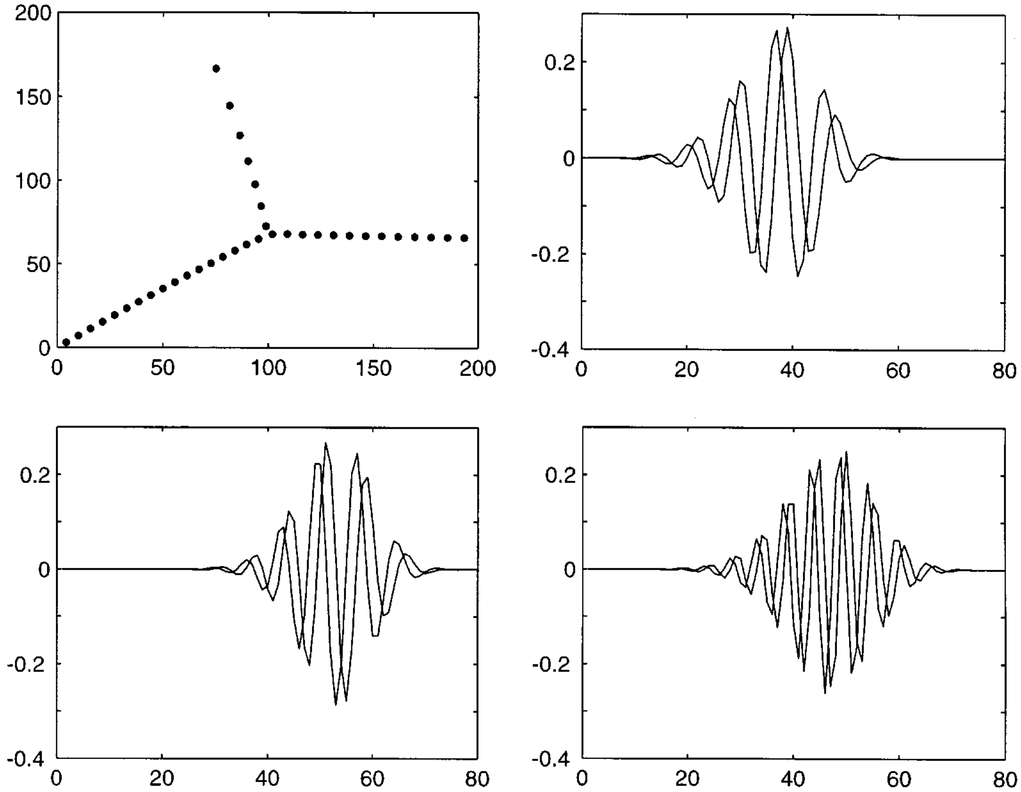

Figure 2. Harmonic oscillator eigenfunctions for various eigenvalues.

for the inside contour. We also plotted the real and imaginary parts of some of the eigenfunctions in figure 2, for $b = 16$ and $m = 20$. The eigenvalues corresponding to these eigenfunctions are approximately $61.5 + 42.9\mathrm{i}$, $86.3 + 126.9\mathrm{i}$ and $201.3 + 65.7\mathrm{i}$. Note the approximately Gaussian form of the eigenfunctions, confirming the formula for f_η in the last section. Finally, we perturbed the operator A slightly by adding ε to all the coefficients $A_{r,s}$ such that $1 \leqslant r = s \leqslant 4m$. It is seen in figure 3, which has $b = 16$ and $m = 20$, that even for $\varepsilon = 10^{-4}$ the eigenvalues at some distance from the origin have a completely different distribution from that without the perturbation.

The peculiar distribution of the large eigenvalues for the unperturbed operator has three explanations. We have discretized the space variable and restricted it to the interval $(0, b)$ so the eigenvalues cannot be exactly the same as those for the harmonic oscillator. However, the results of § 2 demonstrate that the larger eigenvalues are intrinsically unstable, so one should not take seriously the values that we have computed. In effect, it is not possible to compute large eigenvalues numerically, and if a problem of this general type appears to require this, the problem has probably been posed incorrectly.

4. One-sided anharmonic operators

In this section we extend the results of § 2 to a wider class of Schrödinger operators. The ideas involved are similar, but they involve more effort to implement. Let H be

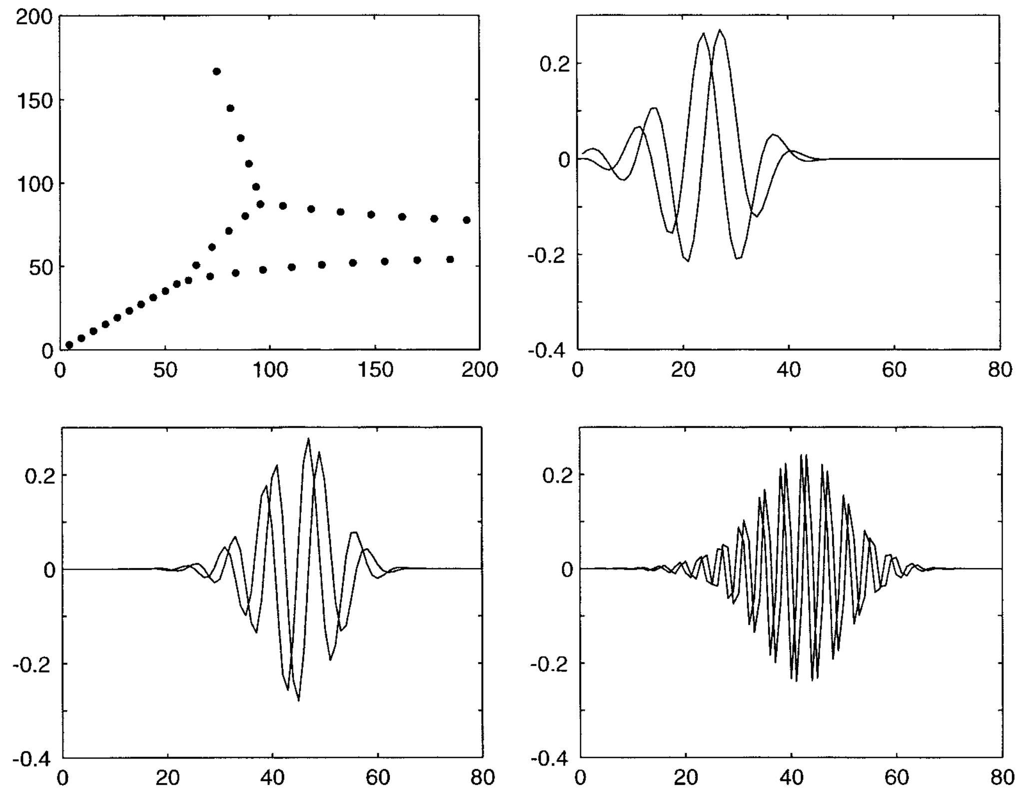

Figure 3. Some eigenvalues and eigenfunctions of the harmonic oscillator with a perturbation of magnitude 10^{-4}.

a densely defined linear operator acting in $L^2(\mathbb{R})$ whose domain contains the space $\mathcal{D} := C_c^\infty(0,\infty)$ of smooth functions with compact support in $(0,\infty)$. Suppose that

$$Hf(x) = -f''(x) + V(x)f(x)$$

for all $f \in \mathcal{D}$ and all $x \in \mathbb{R}$, where V is a locally bounded potential such that

$$\lim_{x\to+\infty}(V(x) - cx^n) = 0$$

for some positive integer n and some constant c such that $\mathrm{Re}(c) > 0$ and $\mathrm{Im}(c) > 0$. We will prove that the norm of the resolvent $(H - zI)^{-1}$ diverges as $|z| \to \infty$ within the sector

$$S := \{z : 0 < \arg(z) < \arg(c)\},$$

where we interpret the norm to be $+\infty$ if z lies in the spectrum of H.

As before we construct JWKB-type test functions f_η, which are smooth truncations of the functions

$$\phi(x) := \mathrm{e}^{-\psi(x)},$$

but now we put $x_0 := \alpha\eta^{2/n}$ and

$$\psi(x_0 + s) := \psi_1 s + \tfrac{1}{2}\psi_2 s^2 + \tfrac{1}{3}\psi_3 s^3 + \tfrac{1}{4}\psi_4 s^4,$$

where $\alpha > 0$ is arbitrary. For the time being we assume that $x := x_0 + s > 0$ and that $V(x) = cx^n$ for all such x. We put

$$\begin{aligned}\psi_1 &:= \mathrm{i}\eta,\\ \psi_2 &:= \frac{V'(x_0)}{2\mathrm{i}\eta} + g\eta^{-4/n},\\ &= f\eta^{1-2/n} + g\eta^{-4/n},\\ \psi_3 &:= h\eta^{1-4/n},\\ \psi_4 &:= k\eta^{1-6/n},\end{aligned}$$

where the constants g, h, k are to be determined, but f is fixed by the above equations. We also put

$$\begin{aligned}z_\eta &:= \psi_2 - \psi_1^2 + V(x_0),\\ &= \eta^2 + V(x_0) + f\eta^{1-2/n} + g\eta^{1-4/n},\\ &= \eta^2(1 + c\alpha^n + f\eta^{-1-2/n} + g\eta^{-2-4/n}),\\ &\sim \eta^2(1 + c\alpha^n),\end{aligned} \tag{4.1}$$

as $\eta \to +\infty$.

Note that for any choice of $\alpha > 0$, z_η lies in the sector S for large enough η, and that any asymptotic direction in this sector may be achieved for a suitable choice of α. We now determine the order of magnitude (in terms of η) of the constants γ_i such that

$$H\phi(x_0 + s) - z_\eta\phi(x_0 + s) = \left(\sum_{i=0}^{\max(6,n)} \gamma_i s^i\right)\phi(x_0 + s).$$

In the calculations below, q_j denote various constants independent of η, and of g, h, k until the values of those constants are chosen. Our choice of z_η yields $\gamma_0 = 0$. Direct calculations show that $\gamma_1 = 0$ if $h = \mathrm{i}g$, and that

$$\gamma_2 = (3k - 2fg)\eta^{1-6/n} - g^2\eta^{-8/n}$$

if $-2\mathrm{i}h - f^2 + q_1 = 0$. We use the above two conditions to fix h and then g. We also have

$$\gamma_3 = -2gh\eta^{1-8/n}$$

if $-2\mathrm{i}k - 2fh + q_2 = 0$, and we use this to fix k. We next observe that

$$\begin{aligned}\gamma_4 &= -2\psi_2\psi_4 - \psi_3^2 + q_3 x_0^{n-4}\\ &= q_4\eta^{2-8/n} - q_5\eta^{1-10/n},\end{aligned}$$

with similar but simpler expressions for other γ_i. The proof of the following lemma is elementary.

Lemma 4.1. *With the above choices of g, h, k we have $\gamma_0 = \gamma_1 = 0$ and*

$$\gamma_i = \mathrm{o}(\eta^{(1/2-1/n)i})$$

for all $i \geqslant 2$.

Our next lemma will provide upper and lower bounds on ϕ, and an upper bound on ϕ'. The proofs are again direct computations.

Lemma 4.2. *If $x_0 + s > 0$ and $\eta > 0$ then*

$$|\operatorname{Re}\psi(x_0+s) - \tfrac{1}{2}\beta s^2\eta^{1-2/n}| \leqslant \tfrac{1}{2}|gs^2|\eta^{-4/n} + \tfrac{1}{3}|hs^3|\eta^{1-4/n} + \tfrac{1}{4}|ks^4|\eta^{1-6/n},$$

where

$$\beta := \operatorname{Re}(f) = \operatorname{Im}(c)n\alpha^{n-1}/2 > 0.$$

Moreover,

$$|\psi'(x_0+s)| \leqslant \eta + |fs|\eta^{1-2/n} + |gs|\eta^{-4/n} + |hs^2|\eta^{1-4/n} + |ks^3|\eta^{1-6/n}.$$

We finally define f_η by

$$f_\eta(x) = p(x)\phi(x), \tag{4.2}$$

where $p \in C_c^\infty(\mathbb{R})$ satisfies $p(x) = 1$ if $|x - x_0| \leqslant \eta^{1/n}$ and $p(x) = 0$ if $|x - x_0| \geqslant 2\eta^{1/n}$. We also require that $|p'(x)| \leqslant q_6\eta^{-1/n}$ and $|p''(x)| \leqslant q_7\eta^{-2/n}$ for all $x \in \mathbb{R}$.

Lemma 4.3. *There exist positive constants a_1 and a_2 such that*

$$a_1\eta^{1/n-1/2} \leqslant \|f_\eta\|^2 \leqslant a_2\eta^{1/n-1/2}$$

for all η that are large enough.

Proof. If η is large enough we have

$$\begin{aligned}
\|f_\eta\|^2 &\geqslant \int_0^{\eta^{1/n}} |\phi(x_0+s)|^2\,\mathrm{d}s \\
&\geqslant \int_0^{\eta^{1/n}} \exp[-\beta s^2\eta^{1-2/n} - q_8 s^2\eta^{-4/n} - q_9 s^3\eta^{1-4/n} - q_{10}s^4\eta^{1-6/n}]\,\mathrm{d}s \\
&= \int_0^1 \exp[-\beta t^2\eta - q_8t^2\eta^{-2/n} - q_9t^3\eta^{1-1/n} - q_{10}t^4\eta^{1-2/n}]\eta^{1/n}\,\mathrm{d}t \\
&\geqslant \int_0^1 \exp[-2\beta t^2\eta]\eta^{1/n}\,\mathrm{d}t \\
&= \eta^{1/n-1/2}\int_0^{\eta^{1/2}} \exp[-2\beta u^2]\,\mathrm{d}u \\
&\geqslant a_1\eta^{1/n-1/2}.
\end{aligned}$$

The proof of the upper bound is similar. ∎

We finally have to estimate

$$\begin{aligned}
Hf_\eta - z_\eta f_\eta &= -(p\phi)'' + Vp\phi - z_\eta p\phi \\
&= p(-\phi'' + V\phi - z_\eta\phi) - 2p'\phi' - p''\phi \\
&= \Big(\sum_i \gamma_i s^i\Big)p\phi + 2p'\psi'\phi - p''\phi.
\end{aligned}$$

Theorem 4.4. *We have*

$$\lim_{\eta\to+\infty} \|Hf_\eta - z_\eta f_\eta\|/\|f_\eta\| = 0,$$

where z_η *is given by (4.1) and* f_η *is given by (4.2). Hence*

$$\lim_{\eta\to+\infty} \|(H - z_\eta I)^{-1}\| = +\infty.$$

Proof. Let χ be the characteristic function of

$$S := \{x_0 + s : \eta^{1/n} \leqslant |s| \leqslant 2\eta^{1/n}\}.$$

Since p' and p'' have supports within S, we have

$$\|Hf_\eta - z_\eta f_\eta\| \leqslant \sum_i |\gamma_i|\, \|s^i p\phi\| + 2q_6\eta^{-1/n}\|\chi\psi'\phi\| + q_7\eta^{-2/n}\|\chi\phi\|,$$

and we have to compare the size of each of these terms with $\|f_\eta\|$ as $\eta \to +\infty$. The last two terms are easy to deal with because ϕ is exponentially small on S. ■

The method of lemma 2.3 yields

$$\begin{aligned}\|s^i p\phi\|^2 &\leqslant \int_{-2\eta^{1/n}}^{2\eta^{1/n}} |s^{2i}| \exp[-\tfrac{1}{2}\beta s^2\eta^{1-2/n}]\,\mathrm{d}s\\ &= O(\eta^{(1/n-1/2)(2i+1)}).\end{aligned}$$

Therefore

$$|\gamma_i|\,\|s^i p\phi\| = o(\eta^{(1/2-1/n)i+(1/n-1/2)(i+1/2)}) = o(\|f_\eta\|).$$

We finally go back to the more general class of potentials considered in the introduction to this section, namely

$$V(x) = cx^n + W(x) \tag{4.3}$$

for all $x \geqslant 0$, where W is bounded and $W(x) \to 0$ as $x \to +\infty$.

Corollary 4.5. *The conclusion of the theorem still holds for potentials of the form (4.3).*

Proof. We need only observe that the support of f_η is contained in $[\alpha\eta^{2/n} - 2\eta^{1/n}, \infty)$ and that W is uniformly small on this interval as $\eta \to +\infty$. ■

5. Complex resonances

We consider the self-adjoint operator H acting in $L^2(\mathbb{R})$, according to the formula,

$$Hf(x) := -f''(x) + kx_+ f(x) + \delta_0 f(x),$$

where δ_0 is the delta function at the origin and $k > 0$ is an arbitrary constant. This operator describes the motion of a quantum particle subject to a reflecting barrier in the right-hand half-line and a partly confining barrier at the origin. Rigorously, H is the non-negative self-adjoint operator associated with the quadratic form,

$$Q(f) := \int_{-\infty}^{+\infty} (|f'(x)|^2 + kx_+|f(x)|^2)\,\mathrm{d}x + |f(0)|^2.$$

If $c > 0$, then H is unitarily equivalent, by a dilation transformation, with the operator,

$$H_{\mathrm{c}} f(x) := -c^{-2} f''(x) + ckx_{+} f(x) + c^{-1}\delta_0 f(x).$$

For complex c such that $\operatorname{Re} c > 0$ and $\operatorname{Im} c > 0$, the operator has complex eigenvalues, which are independent of c and which are called complex resonances of H. These resonances are uncovered by the continuous spectrum $c^{-2}[0,\infty)$ of H_{c} as the imaginary part of c increases. The real parts of the resonances are close to the eigenvalues of the operator

$$Kf(x) := -f''(x) + kxf(x)$$

acting in $L^2(0,\infty)$ subject to Dirichlet boundary conditions at $x = 0$ (see Aguilar & Combes 1971; Balslev & Combes 1971; Cycon *et al*. 1987; Simon 1973, and references therein).

The theory that we have developed in the previous section applies to the operator $c^2 H_{\mathrm{c}}$ and implies that the pseudo-spectra of H_{c} fill out the sector $\{z : -2\arg c < \arg z < \arg c\}$. Thus any resonances in this sector that are not close to the origin are intrinsically unstable under small perturbations of the operator H. This is not merely a problem at very high energies. We have done numerical studies of a discrete approximation to this problem, defined as follows. The positive integer h below represents the number of points replacing each unit interval of the original problem, while $-a$ and b represent space cut-offs on the left and right of the origin, respectively.

Let A be the $h(a+b)\times h(a+b)$ matrix whose entries are

$$A_{r,s} := \begin{cases} w(r), & \text{if } r = s,\\ -c^{-2}h^2, & \text{if } r - s = \pm 1,\\ 0, & \text{otherwise,}\end{cases}$$

where

$$w(r) := \begin{cases} 2c^{-2}h^2 + ck(r - ah)/h, & \text{if } r > ah,\\ 2c^{-2}h^2 + c^{-1}h, & \text{if } r = ah,\\ 2c^{-2}h^2, & \text{otherwise.}\end{cases}$$

We have computed the spectrum and level curves of the pseudo-spectra of this operator for various values of a, b, h, k, c using MATLAB. The smallest singular value σ_z of $H - zI$ is equal to the inverse of the norm of the resolvent operator $R := (H - zI)^{-1}$. Since σ_z is very small for the values of z we have examined, and A is a tridiagonal matrix, inverse iteration is a very efficient technique. We have

$$\|R\| \geqslant \|R(R^*R)^m u\| / \|(R^*R)^m u\|$$

for any initial vector u and any non-negative integer m, and we have found that good approximations are obtained with $u = \text{const.}$ and $m = 1$. For our purposes, which are simply to demonstrate that $\|R\|$ may be very large far from the spectrum, any large enough lower bound on the resolvent norm suffices, and we do not need to worry about the possibility that the norm may be even larger than that computed.

In figure 4 we have put $a = 20$, $b = 20$, $h = 10$, $k = 5$ and $c = 1 + 0.1\mathrm{i}$. The level curves were constructed by MATLAB using a uniform 50×50 grid of evaluations of the resolvent norm. The eigenvalues on the sloping line through the

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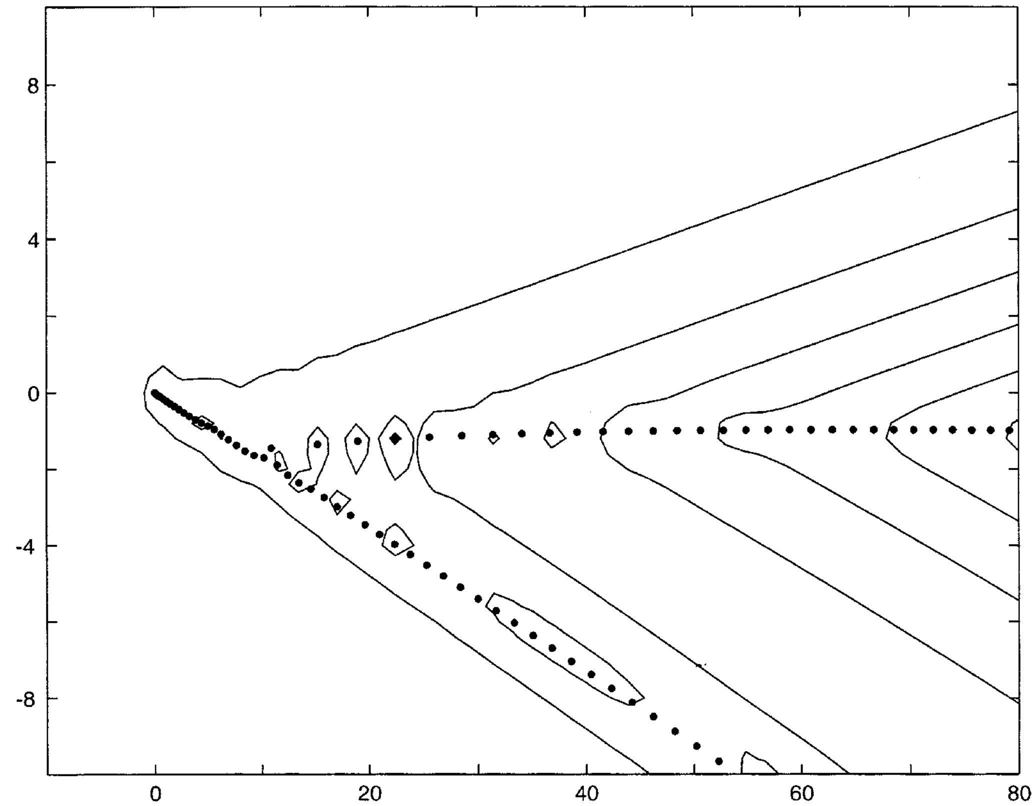

Figure 4. Resonances near the real axis of a Schrödinger operator with the associated pseudo-spectra.

origin represent the continuous spectrum of the operator H_c, while the eigenvalues on the roughly horizontal curve below the x-axis are the resonances. There are many further eigenvalues outside the diagram, but their positions are dependent on the particular discretization and space cut-offs chosen. The diagram also shows the level curves where the resolvent norm equals 10^m for some integer $m \geqslant 0$, starting from the outside curve with $m = 0$.

The numerical data confirm that the resolvent norms diverge to $+\infty$ along rays within the sector. The rate of divergence is remarkably fast, and we conjecture that the resolvent norms grow exponentially as $\eta \to +\infty$. The size of the resolvent norms and the general theory of pseudo-spectra suggest that only the first 30 or so resonances are effectively computable if one works within the context of dilation analyticity and L^2 theory.

The instability of the spectrum far from the origin is proved by our asymptotic theorems combined with (1.1), but may also be illustrated numerically. In figure 5 we have recomputed the spectrum and pseudo-spectra when one adds $10^{-3}\sin(r)$ to the potential for $1 \leqslant r \leqslant h(a+b)$. The first 16 resonances (counting according to their absolute values) are only slightly affected, but larger resonances are in quite different positions from those of figure 4. Note, however, that the pseudo-spectral contours are much less affected by the perturbation, as the theory predicts.

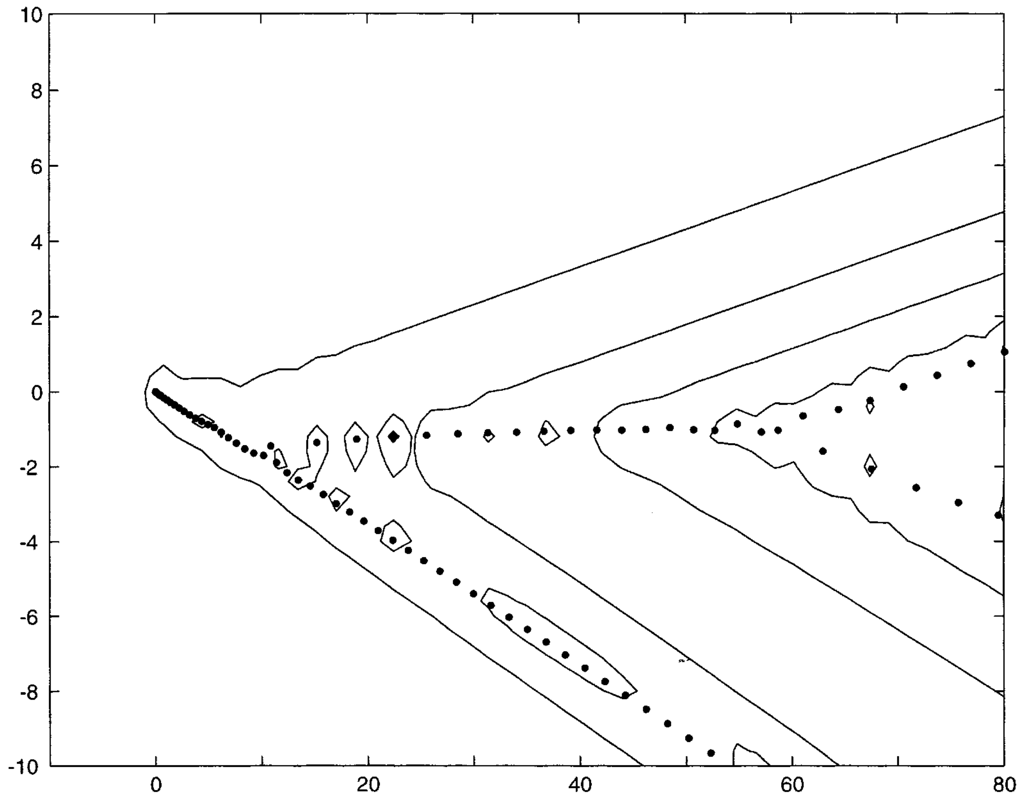

Figure 5. Eigenvalues and pseudo-spectra of the resonance model with a perturbation of magnitude 10^{-3}.

The implications of these results for the general theory of complex resonances are substantial. Many definitions of complex resonance depend upon analytic continuation arguments. While analytic continuations are guaranteed to be unique if they exist, they are also hard to compute because of their inherent instability: arbitrarily small perturbations of an analytic function within a region can lead to large movements of poles of its analytic continuation outside that region. Unless a physical problem imposes and a computational procedure makes use of inherent restrictions on the type of perturbation allowable, one should be cautious about its significance in resonance theory.

I thank M. Brown for questions that led me to start this work, and L. N. Trefethen for helpful comments.

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