BOUNDS ON COMPLEX EIGENVALUES AND RESONANCES

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ABSTRACT. We obtain bounds on the complex eigenvalues of non-self-adjoint Schrödinger operators with complex potentials, and also on the complex resonances of self-adjoint Schrödinger operators. Our bounds are compared with numerical results, and are seen to provide useful information.

1. INTRODUCTION

We consider self-adjoint and non-self-adjoint Schrödinger operators of the form

$$Hf := -\Delta f + Vf$$

acting in $L^2(\mathbf{R}^N)$, where V is a potential vanishing sufficiently rapidly as $|x| \to \infty$. When V is a complex-valued potential we obtain bounds on the location of the eigenvalues of H, while in the case when V is real-valued we obtain bounds on its resonances. We also describe and implement methods for computing eigenvalues and resonances, and compare them both with each other and with others.

There appears to be rather little literature on either of these problems. The distribution of the eigenvalues of self-adjoint Schrödinger operators has been intensively studied for several decades, but most of the techniques are not applicable to non-self-adjoint operators. Similarly most of the literature concerning resonances is either computational or considers the semi-classical limit and resonances close to the real axis. Our results are of quite a different character.

The principal technique which we use to obtain bounds on eigenvalues and resonances in sections 2 and 4 involves obtaining constraints on the numerical range of the operator H and of others closely related to it. In section 3, however, we describe a quite different technique

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for ordinary differential operators which yields similar bounds but also enables us to prove that the number of eigenvalues of such operators is finite for potentials which decay rapidly enough. Section 5 is devoted to obtaining a first order perturbation formula for resonances of a Schrödinger operator. For a general perturbation theory of resonances see, for instance, [1] and references therein.

The remaining two sections concentrate on the computation of resonances. We have investigated such problems using a well-known complex scaling method for Schrödinger operators with dilation analytic potentials elsewhere [2], but here we consider Schrödinger operators in one dimension with rapidly decaying potentials which need not be analytic. In section 6 we describe two different methods of computing the resonances of such operators. In the final section 7 of the paper we apply our results to several examples. In particular, for comparison purposes we take operators for which the location of the resonances has already been determined. One of the examples of section 7 dates back to the series of papers [9, 7, 8], another to our earlier paper [2]. We find that the two methods of section 6 have similar accuracy, but these methods are sometimes a lot much useful than the complex scaling method and sometimes considerably less accurate. In all cases the key numerical issue is the accurate computation of highly oscillatory integrals.

2. Bounds on eigenvalues using complex scaling

We initially assume for simplicity that V is a bounded complex-valued potential such that $V(x) \to 0$ as $|x| \to \infty$. Since V is then a relatively compact perturbation of $-\Delta$ it follows routinely from [6] that the spectrum of H consists of $\mathbf{R}^+ := [0, \infty)$ together with a finite or countable number of eigenvalues of finite multiplicity which can only accumulate at points of $\mathbf{R}^+$.

We also assume that $z \to V(zx)$ is complex analytic for all $x \in \mathbf{R}^N$ and all z in the closed sector

$$\{z \in \mathbf{C} : 0 \leq 2\arg(z) \leq \alpha\}$$

where $0 < \alpha \leq \pi$ and $V(zx) \to 0$ as $|x| \to 0$ uniformly with respect to z in compact subsets of the sector. We then put

$$c(\theta) := \|V(\mathrm{e}^{i\theta/2}\cdot)\|_\infty$$

for all θ satisfying $0 \leq \theta \leq \alpha$. It follows from the three lines lemma that $c(\theta)$ is a logarithmically convex function of θ. In the theorem below and elsewhere we adopt the notation

$$B(a, r) := \{z \in \mathbf{C} : |z - a| \leq r\}.$$

Theorem 1. *Under the above assumptions on V the eigenvalues λ of H which do not satisfy $-\alpha \leq \arg(\lambda) \leq 0$ all lie in the compact convex* *set*

$$\bigcap_{0\le\theta\le\alpha} \left\{ \mathrm{e}^{-i\theta}\mathbf{R}^+ + B(0,c(\theta)) \right\}$$

and their only possible accumulation point is at 0*.*

Proof. If we put

$$\hat{H}_z := -z^{-2}\Delta + V(z\,\cdot)$$

then $\hat{H}_z$ is unitarily equivalent to H for positive real z, so its eigenvalues are independent of z. The same applies by analytic continuation for complex z, in a sense which is familiar in the theory of resonances [4, 5]. When

$$H_\theta := -\mathrm{e}^{-i\theta}\Delta + V(\mathrm{e}^{i\theta/2}\,\cdot)$$

for $0 \le \theta \le \alpha$ then the essential spectrum of H_θ depends on θ, being equal to $\mathrm{e}^{-i\theta}\mathbf{R}^+$. Since the eigenvalues can only accumulate in the essential spectrum and the only common point of the essential spectra of all of these operators is 0, this is the only possible limit point of the eigenvalues.

In order to obtain bounds on the position of the eigenvalues, we need to introduce the numerical range

$$\mathrm{Num}(\theta) = \left\{ \langle H_\theta f, f\rangle : \|f\| = 1 \right\},$$

where we assume that all f lie in the θ-independent domain of H_θ. In the current situation $\mathrm{Num}(\theta)$ is a convex set which contains the entire spectrum of H_θ and is contained in

$$\mathrm{e}^{-i\theta}\mathbf{R}^+ + B(0,c(\theta)).$$

It follows that if λ is an eigenvalue of H then λ lies in this set for all $0 \le \theta \le \alpha$. ☐

Note If the sector of analyticity of V contains the positive real axis in its interior, then under similar assumptions one concludes that the only possible accumulation point of the set of *all* eigenvalues is 0.

Other bounds of a similar type are available, depending on what information about the potential one wishes to use.

Theorem 2. *Under the above assumptions on* V *the eigenvalues* λ *of* H *which satisfy* $\mathrm{Im}(\lambda) > 0$ *all lie in the closed convex set*

$$\bigcap_{0\le\theta\le\alpha} \left\{ x+iy : x\sin(\theta) + y\cos(\theta) \le a(\theta) \right\},$$

where the convex function $a(\cdot)$ *on* $[0,\alpha]$ *is defined by*

$$a(\theta) := \sup\left\{ \mathrm{Im}(\mathrm{e}^{i\theta}V(\mathrm{e}^{i\theta/2}v)) : v \in \mathbf{R}^N \right\}.$$

Proof. The main statement of the theorem depends upon the fact that

$$\mathrm{Num}(\theta) \subseteq \{x+iy : x\sin(\theta)+y\cos(\theta) \le a(\theta)\}\ .$$

We now explain why $a(\cdot)$ is convex. If we define

$$g(z,v) := \mathrm{Im}\{z^2 V(zv)\}$$

for $0 \le 2\arg(z) \le \alpha$, then as the real part of an analytic function $g(\cdot,v)$ is harmonic. Hence

$$h(z) := \sup\{g(z,v) : v \in \mathbf{R}^N\}$$

is subharmonic and constant on each ray through the origin. This forces $a(\cdot)$ to be convex. □

It is clear that similar bounds can be obtained for certain unbounded potentials. In the next theorem we state a general result of this type which uses quadratic form techniques. Here we make the same assumptions on the analyticity of V in the sector as before, but replace the regularity assumptions as indicated.

Theorem 3. *Suppose that $V_\theta := V(\mathrm{e}^{i\theta/2}\,\cdot)$ is relatively compact with respect to $-\Delta$ for all $0 \le \theta \le \alpha$, and that for all such θ the operator inequality*

$$|V_\theta| \le \gamma_\theta(-\Delta) + \beta_\theta$$

holds where $0 \le \gamma_\theta < 1$. Then every eigenvalue λ of H which does not satisfy $-\alpha \le \arg(\lambda) \le 0$ lies in the closed convex set

$$\bigcap_{0\le\theta\le\alpha} \{C_\theta + B(0,\beta_\theta)\}\ ,$$

where

$$C_\theta := \{z : -\theta - \arcsin(\gamma_\theta) \le \arg(z) \le -\theta + \arcsin(\gamma_\theta)\}\ .$$

Proof. The only new component of the proof is the observation that if we put $s := \langle -\Delta f, f\rangle$ then we obtain

$$\begin{aligned} \mathrm{Num}(H_\theta) &\subseteq \bigcup_{s\in\mathbf{R}^+} B(\mathrm{e}^{-i\theta}s, \sin(\gamma_\theta)s+\beta_\theta) \\ &= C_\theta + B(0,\beta_\theta). \end{aligned}$$

□

3. Resolvent bounds on complex eigenvalues

This section describes a completely different assumption under which one can obtain bounds on the complex eigenvalues, at least in one dimension. We replace the analyticity assumption on the potential V by the assumption that V lies in $L^1(\mathbf{R})\cap L^2(\mathbf{R})$. This is known to imply that V is a relatively compact perturbation of $-\Delta$ acting in $L^2(\mathbf{R})$, so the spectrum of $H = -\Delta + V$ is again equal to $\mathbf{R}^+$ together with eigenvalues which can only accumulate on the non-negative real axis. Moreover the domain of H is equal to $W^{2,2}(\mathbf{R})$, which is contained in $C_0(\mathbf{R})$.

Theorem 4. *Under the above assumptions every eigenvalue λ of H which does not lie on the positive real axis satisfies*

$$|\lambda| \leq \|V\|_1^2/4.$$

Proof. Let $\lambda = -z^2$ be an eigenvalue of H where $\operatorname{Re} z > 0$ and let f be the corresponding eigenfunction, so that $f \in C_0(\mathbf{R})$. Then

$$(-\Delta + z^2)f = -Vf \tag{1}$$

so

$$-f = (-\Delta + z^2)^{-1}Vf.$$

Putting $X := |V|^{1/2}$, $W := V/X$ and $g := Wf \in L^2$, we deduce that

$$-g = W(-\Delta + z^2)^{-1}Xg \tag{2}$$

so

$$-1 \in \operatorname{Spec}(W(-\Delta + z^2)^{-1}X).$$

This approach is similar to the Birman–Schwinger principle for finding eigenvalues of self-adjoint operators (see, for instance, [3]). By evaluating the Hilbert-Schmidt norm of the above operator, whose kernel is

$$W(x)\frac{\mathrm{e}^{-z|x-y|}}{2z}X(y)$$

we deduce that

$$\int_{\mathbf{R}^2} |W(x)|^2 \frac{\mathrm{e}^{-2\operatorname{Re} z|x-y|}}{4|z|^2} |X(y)|^2 \mathrm{d}x\mathrm{d}y \geq 1.$$

This implies $\|V\|_1^2/4|z|^2 \geq 1$. ☐

It appears more difficult to prove that the number of eigenvalues of H is finite or to obtain bounds on the number. The following theorem which treats the operator H in one dimension provides a result of this kind.

Theorem 5. *Let the potential V satisfy*

$$\|V(x)\mathrm{e}^{\gamma x}\|_1 < \infty \tag{3}$$

for all $\gamma \in \mathbf{R}$. Then the number of the eigenvalues of H is finite and all the eigenvalues (including real ones) satisfy

$$|\lambda| \le \frac{9}{4}\|V\|_1^2.$$

Proof. Along with (1) consider the equation

$$u'' - z^2 u = 0.$$

Its linearly independent solutions are

$$u_1(x) = \frac{\sinh(zx)}{z}, \qquad u_2(x) = \cosh(zx).$$

We shall seek the solution $f(x)$ of (1) in the form

$$f(x) = C_1(x)u_1(x) + C_2(x)u_2(x),$$

where the functions C_1, C_2 satisfy

$$C_1'(x) = V(x)f(x)\cosh(zx), \qquad C_2'(x) = -V(x)f(x)\frac{\sinh(zx)}{z}.$$

We take $C_1(-\infty) = z$, $C_2(-\infty) = 1$ which corresponds to $f(x) \sim \mathrm{e}^{zx}$, $x \to -\infty$. Then

$$C_1(x) = z + \int_{-\infty}^{x} V(t)f(t)\cosh(zt)\,\mathrm{d}t,$$

$$C_2(x) = 1 - \int_{-\infty}^{x} V(t)f(t)\frac{\sinh(zt)}{z}\,\mathrm{d}t.$$

It follows from (3) that

$$\lim_{x\to+\infty} |C_k(x)| < \infty, \qquad k = 1, 2.$$

We define the function

$$\varphi(z) = C_1(\infty) + zC_2(\infty). \tag{4}$$

As is easily seen,

$$\varphi(z) = 2z + \int_{\mathbf{R}} V(t)\tilde{f}(t)\mathrm{d}t, \tag{5}$$

where

$$\tilde{f}(x) = f(x)\mathrm{e}^{-zx} = 1 + \frac{1}{2z}\int_{-\infty}^{x}\left(1 - \mathrm{e}^{-2z(x-t)}\right)V(t)\tilde{f}(t)\mathrm{d}t.$$

We observe that if $\lambda = -z^2$ is an eigenvalue of H, then $\varphi(z) = 0$, $\operatorname{Re} z \ge 0$. For z in the right-hand half-plane we have

$$\left|1 - \mathrm{e}^{-2z\tau}\right| \le 2 \qquad \forall\tau > 0$$

and, hence

$$|\tilde{f}(x)| \le 1 + \frac{1}{|z|}\int_{-\infty}^{x} |V(t)\tilde{f}(t)|\mathrm{d}t.$$

From this formula we get

$$\sup_{x\in\mathbf{R}} |\tilde{f}(x)| \le \frac{|z|}{|z| - \|V\|_1}.$$

This together with (5) implies

$$\varphi(z) = 2z + \psi(z), \qquad |\psi(z)| \le \frac{|z|\|V\|_1}{|z| - \|V\|_1}.$$

Therefore $\varphi(z) \ne 0$ for sufficiently large $|z|$. In particular, if $|z| > \frac{3}{2}\|V\|_1$ then $|\psi(z)| < 2|z|$ and $\varphi(z) \ne 0$ for all such z.

Since $\tilde{f}(x; z)$ is analytic in z, the function φ defined by (4) is entire. Therefore the number of its zeros in any bounded domain is finite. The eigenvalues of H can only be found among the squares of the zeros of $\varphi(z)$, hence the final result. □

Note Bounds similar to those in the above two theorems can be obtained for the corresponding operator on the half-line subject to the boundary condition $af(0) + bf'(0) = 0$, $|a| + |b| > 0$, by minor adjustments to the proof.

4. Complex scaling and resonance bounds

We now apply the above results to the analysis of the complex resonances of a self-adjoint Schrödinger operator H. We assume that V is real-valued, and that it can be analytically continued to the closed sector $\{z : -\alpha \le \arg(z) \le 0\}$ with the same bounds on V_θ as in theorem 1. H itself has no complex eigenvalues but well-known arguments [4, 5] show that those eigenvalues of H_θ which lie within the sector

$$\{z : -\theta < \arg(z) \le 0\}$$

are independent of θ. New eigenvalues may be emerge from the essential spectrum $\mathrm{e}^{-i\theta}\mathbf{R}^+$ as θ increases. The set of all such eigenvalues as θ varies over the permitted range is called the set of resonances of H. It is known that this definition is equivalent to others which do not depend upon complex scaling.

We assume that V_θ is bounded and vanishes at infinity for all θ in the permitted range and put

$$a(\theta) := \sup\left\{\mathrm{Im}(\mathrm{e}^{i\theta}V(\mathrm{e}^{i\theta/2}v)) : v \in \mathbf{R}^N\right\}$$

as before.

Theorem 6. *Under the above assumptions those resonances of H which satisfy $-\alpha < \arg(z) \le 0$ all lie within the closed convex set*

$$S := \bigcap_{0\le\theta\le\alpha} \{x + iy : x\sin(\theta) + y\cos(\theta) \le a(\theta)\}.$$

Proof. Given θ, every resonance in the stated sector either has not yet been uncovered, in which case $-\alpha \le \arg(z) \le -\theta$, or it has been uncovered, in which case

$$x \sin(\theta) + y \cos(\theta) \le a(\theta).$$

The proof is completed by a geometrical argument. The set S is the intersection of half-planes, and hence is closed and convex. $\square$

The boundary of the set S is the envelope of the lines

$$x \sin(\theta) + y \cos(\theta) = a(\theta).$$

which is given parametrically by

$$\begin{aligned} x &= a(\theta)\sin(\theta) + a'(\theta)\cos(\theta) \\ y &= a(\theta)\cos(\theta) - a'(\theta)\sin(\theta). \end{aligned}$$

We use this formula to find the form of the envelope as it emerges from the real axis.

Theorem 7. *If $a(\theta) = a_1\theta + a_2\theta^2 + O(\theta^3)$ for small $\theta > 0$ then $a_1 \ge 0$ and $a_2 \ge 0$. Assuming $a_2 > 0$, the form of the envelope of S is*

$$y = -\frac{(x - a_1)^2}{4a_2} + o((x - a_1)^2)$$

for $(x - a_1)$ small and positive.

Proof. An application of Taylor's theorem shows that

$$a_1 = \max\{V(x) + x \cdot \nabla V(x)/2 : x \in \mathbf{R}^N\}$$

and this implies that

$$a_1 \ge M := \max\{V(x) : x \in \mathbf{R}^N\} \ge 0.$$

The inequality $a_2 \ge 0$ follows from the fact that the function $a(\cdot)$ is convex. The main statement of the theorem depends upon eliminating θ from the formulae

$$\begin{aligned} x &= a_1 + 2a_2\theta + O(\theta^2) \\ y &= -a_2\theta^2 + O(\theta^3). \end{aligned} \tag{6}$$

$\square$

Note While one expects the hypothesis $a_2 > 0$ of the above theorem to hold generically, the example of subsection 7.2 has $a_2 = 0$, and a higher order expansion would be needed to determine the form of the envelope near the real axis.

Physical intuition suggests that there cannot be resonances λ with $\mathrm{Im}(\lambda)$ very small and $\mathrm{Re}\,\lambda > M$, which is confirmed by the example of subsection 7.2 (see figure 1), where $\mathrm{Re}\,\lambda < M \approx 36.79$. However, theorem 7 fails to prove quite as much. In the case in which $V(x) =$

$x^2\mathrm{e}^{-x^2/b^2}$ for some $b > 0$, a simple computation shows that $a_1/M \sim 1.256$.

A threshold for the resonances of an operator H is defined to be a real number γ such that every resonance λ of H satisfies $\operatorname{Re}\lambda \le \gamma$.

Corollary 8. *If $\alpha \ge \pi/2$ then the resonances of the operator H possess a threshold.*

Proof. On choosing $\theta = \pi/2$, we see that every resonance satisfies $\operatorname{Re}\lambda \le a(\pi/2)$. ☐

Corollary 9. *Let $r = 1$ or 2 and let*

$$V(x) = \int_{\mathbf{R}^+} \mathrm{e}^{-s|x|^r}\mu(\mathrm{d}s)$$

for all $x \in \mathbf{R}^N$, where μ is a finite signed measure on $\mathbf{R}^+$. Then

$$\gamma = \int_{\mathbf{R}^+} |\mu|(\mathrm{d}s)$$

is a threshold for the resonances of the operator H.

5. Perturbation formulae for resonances

To obtain perturbation formulae let us assume that $V(x)$ is real-valued and positive and rewrite the integral equation (2) as

$$-g(x) = \int_{\mathbf{R}^N} W(x)G(x,y;z)W(y)g(y)\mathrm{d}y,$$

where for all x, y the Green's function $G(x,y;z)$ is analytic in z, $\operatorname{Re} z > 0$, positive for $z > 0$ and satisfies $G(x,y;\bar{z}) = \bar{G}(x,y;z)$. For certain values of N the kernel of (2) is known; the argument below does not use the explicit form of G. The above formula defines the operator

$$A(z)g = \int_{\mathbf{R}^N} W(x)G(x,y;z)W(y)g(y)\mathrm{d}y + g.$$

The resonances therefore are defined as such values of $\lambda = -z^2$ that 0 is an eigenvalue of $A(z)$. The operator $A(z) - I$ has a symmetric kernel for all z, $\operatorname{Re} z \ge 0$, and is self-adjoint for positive real z. However, since we want to consider complex z let us decompose the operator A and the function g as

$$A = A_1 + iA_2, \qquad g = g_1 + ig_2,$$

where the real and imaginary parts $A_{1,2}$ of A are self-adjoint, and $g_{1,2}$ are real-valued. The (non-linear in z) problem

$$A(z)g = 0 \tag{7}$$

is equivalent to the equation

$$\begin{pmatrix} -A_2 & A_1 \\ A_1 & A_2 \end{pmatrix}\begin{pmatrix} g_2 \\ g_1 \end{pmatrix} = 0. \tag{8}$$

The problem (8) involves a family of *self-adjoint* operators so we can now use standard perturbation theory techniques valid for such operators.

Suppose we have a resonance $\lambda_0 = -z_0^2$, i.e. if we put $z = z_0$ in (7) the problem has a solution g_0. Consider a perturbed operator $\hat{A}(z,\varepsilon) = A(z) + \varepsilon B(z) + O(\varepsilon^2)$ obtained, for instance, if we replace V by $V_\varepsilon = V + \varepsilon V_1 + O(\varepsilon^2)$ in (1) (examples are to be found in section 7). Let us find the relevant resonance $\lambda = -z^2$ assuming that $z = z_0 + O(\varepsilon)$. The latter assumption is justified by the above reasoning and by the fact that the operator function $A(z)$ is analytic in z when $z \neq 0$. It is therefore expanded in powers of $(z - z_0)$: $A(z) = A(z_0) + A'(z_0)(z - z_0) + \ldots$; the same is true for $B(z)$. Following the conventional approach (cf. [6]) we seek a solution of the problem $\hat{A}g = 0$ in the form

$$(A(z) + \varepsilon B(z))(g_0 + \varepsilon g_1) = O(\varepsilon^2).$$

Denote $z - z_0 = \varepsilon\nu + O(\varepsilon^2)$. Then the above equation can be rewritten as

$$(A(z_0) + \varepsilon A'(z_0)\nu + \varepsilon B(z_0))(g_0 + \varepsilon g_1) = O(\varepsilon^2)$$

yielding

$$\nu = -\frac{(B(z_0)g_0, g_0)}{(A'(z_0)g_0, g_0)} \tag{9}$$

(here we use the property $Ag = 0 \;\Rightarrow\; A^*\bar{g} = 0$). The operators involved are easily computed as

$$A'(z)g = \int_{\mathbf{R}^N} W(x)\frac{\partial G(x,y;z)}{\partial z}W(y)g(y)\mathrm{d}y,$$

$$B(z)g = \int_{\mathbf{R}^N} V_1(x)G(x,y;z)W(y)g(y)\mathrm{d}y + \int_{\mathbf{R}^N} W(x)G(x,y;z)V_1(y)g(y)\mathrm{d}y.$$

Finally, we formulate the main result of this section.

Theorem 10. *Let λ_0 be a resonance of $H = -\Delta + V$. Then the corresponding resonance of the perturbed operator $H + \varepsilon V_1$*

$$\lambda = \lambda_0 - 2\nu\sqrt{-\lambda_0}\,\varepsilon + O(\varepsilon^2),$$

ν being given by (9) provided the denominator is non-zero.

The first order correction to a given resonance is computed in terms of the solution of the corresponding unperturbed problem similarly to the well-known self-adjoint eigenvalue problem situation. Naturally, (9) involves A' since the problem is non-linear with respect to z.

The above approach essentially uses the symmetry of the kernel of A in the sense that (7) is reduced to the self-adjoint problem, which allows us to compute the correction ν explicitly. However, a similar argument applies in a generic situation. Suppose, we have a non-self-adjoint analytic family of operators $\hat{A}(z,\varepsilon)$ whose simple eigenvalues $\lambda(z,\varepsilon)$ are analytic functions of the two complex variables (see [6], Ch. VII, §4). To find the resonance of the operator $\hat{A}$ we put $\lambda(z,\varepsilon)=0$; this equation can be resolved as $z=z(\varepsilon)$ provided $\frac{\partial\lambda}{\partial z}\neq 0$ by the complex analogue of the implicit function theorem. We therefore conclude that the resonance z depends analytically on the small parameter ε.

Perturbation formulae for a general analytic operator family are derived in [1], where the so-called resonance–eigenvalue connection is established in a very abstract context. In section 7 the author introduces an operator whose eigenvalues coincide with the resonances of the initial operator; then in section 8 the perturbation formulae are obtained along the lines of [6]. We, on the other hand, deal with the particular case of the Schrödinger operator, computing the first order term. The proof of theorem 10, being fairly simple, permits one to switch to the self-adjoint problem, which is advantageous from the practical point of view when one wants to find the correction ν.

6. Rapidly decaying potentials

We describe a technique for finding resonances which depends on rapid decay of the potential instead of analyticity assumptions. The method only works in one space dimension. We treat operators acting in $L^2(\mathbf{R}^+)$ subject to generic boundary conditions at 0; similar methods apply on the whole line.

6.1. Existence and uniqueness of the resonance solution.

Resonances are conventionally defined to be solutions of the singular boundary value problem

$$f''-(V(x)+z^2)f=0, \qquad x\in\mathbf{R}^+ \tag{10}$$

$$af(0)+bf'(0)=0, \qquad |a|+|b|>0, \tag{11}$$

$$f(x)=\mathrm{e}^{zx}+o(|\mathrm{e}^{-zx}|), \qquad x\to\infty \tag{12}$$

Here z is a complex parameter and $V(x)$ is a complex-valued function decaying rapidly enough at infinity:

$$\int_{\mathbf{R}^+}|V(x)|\mathrm{e}^{2zx}\mathrm{d}x<\infty. \tag{13}$$

Lemma 11. *For all z such that $\operatorname{Re} z>0$ there exists exactly one solution of (10) satisfying (12).*

Proof. Denote

$$g(x)=f(x)-\mathrm{e}^{zx},$$

then

$$g''-(V(x)+z^2)g=V(x)\mathrm{e}^{zx}.$$

Let $u_-(x)$, $u_+(x)$ be two linearly independent solutions of (10) defined by

$$u_\pm(x) \sim d_\pm \mathrm{e}^{\pm zx}, \qquad x \to \infty, \tag{14}$$

$d_\pm$ being some constants.

We look for the function $g(x)$ in the form

$$g(x) = C_-(x)u_-(x) + C_+(x)u_+(x),$$

where the functions C_-, C_+ solve

$$C'_-u_- + C'_+u_+ = 0,$$

$$C'_-u'_- + C'_+u'_+ = V(x)\mathrm{e}^{zx}.$$

In other words,

$$C_\pm(x) = \mp\frac{1}{W}\int_x^\infty V(t)\mathrm{e}^{zt}u_\mp(t)\mathrm{d}t. \tag{15}$$

Here the Wronskian $W = \begin{vmatrix} u_- & u_+ \\ u'_- & u'_+ \end{vmatrix}$ is constant. Assumptions (13) and (14) guarantee the convergence of the integrals in (15) and imply

$$|C_+(x)| = o(\mathrm{e}^{-2zx}), \qquad |C_-(x)| = o(1), \qquad x \to \infty.$$

This, in turn, means that

$$g(x) = o(\mathrm{e}^{-zx}), \qquad x \to \infty \tag{16}$$

as required. The way we construct this solution also implies its uniqueness. □

Now that the lemma is proved we are led to the following problem: find such values of z that the equation (10) has a solution satisfying both of the boundary conditions (11) and (12). The values of $\lambda = -z^2$ are the resonances of our problem.

6.2. **First method.** Given any z we can compute at $x = 0$ the value of $g(x; z)$ satisfying (16). The resonances are determined by

$$a(1 + g(0; z)) + b(z + g'(0; z)) = 0. \tag{17}$$

The resonance solution $f(x; z)$ then satisfies the boundary condition (11).

One possible method of evaluating $g(0)$, $g'(0)$ is as follows. Denote

$$\alpha_\pm(x) = u'_\pm(x)/u_\pm(x) \mp z.$$

These two functions can be easily computed as the solutions of the Cauchy problems

$$\alpha'_\pm + \alpha^2_\pm \pm 2\alpha_\pm z - V = 0, \tag{18}$$

$$\alpha_-(\infty) = 0, \qquad \alpha_+(0) = \alpha_0. \tag{19}$$

Here the solutions of the problems (18), (19) are assumed to be bounded on $(0,\infty)$. We then have

$$u_-(x) = u_-(0)\exp\left(\int_0^x \alpha_-(t)\mathrm{d}t - zx\right)$$

and, hence

$$C_+(x) = -W^{-1}u_-(0)\exp\left(\int_{\mathbf{R}^+} \alpha_-(t)\mathrm{d}t\right) I_+(x), \tag{20}$$

where

$$I_+(x) = \int_x^\infty V(t)\exp\left(-\int_t^\infty \alpha_-(\tau)\mathrm{d}\tau\right)\mathrm{d}t.$$

Similarly,

$$C_-(x) = W^{-1}u_+(0)I_-(x) \tag{21}$$

where

$$I_-(x) = \int_x^\infty V(t)\exp\left(2zt + \int_0^t \alpha_+(\tau)\mathrm{d}\tau\right)\mathrm{d}t.$$

A simple calculation gives us

$$W = u_-(0)u_+(0)(\alpha_+(0) - \alpha_-(0) + 2z).$$

We can now evaluate $g(0)$ and $g'(0)$ using (20), (21). The final formulae are

$$g(0) = \frac{I_-(0) - I_+(0)\exp(\int_{\mathbf{R}^+}\alpha_-(x)\mathrm{d}x)}{\alpha_0 - \alpha_-(0) + 2z}, \tag{22}$$

$$g'(0) = \frac{I_-(0)(\alpha_-(0) - z) - I_+(0)(\alpha_0 + z)\exp(\int_{\mathbf{R}^+}\alpha_-(x)\mathrm{d}x)}{\alpha_0 - \alpha_-(0) + 2z}. \tag{23}$$

We did not specify the initial value $\alpha_+(0)$ in (18); now it is clear that we can take any $\alpha_0 \neq \alpha_-(0) - 2z$. Computing $g(0)$, $g'(0)$ by formulae (22), (23) for a range of z we then solve the equation (17) by a standard iterative procedure and, finally find the resonances.

Following this procedure we have to integrate (18), (19) numerically. The equation for α_- is solved from right to left, for α_+ from left to right, which means the integration is stable in both cases. As we compute $\alpha_\pm$, at each integration step the integrals $\int_0^x \alpha_+(t)\mathrm{d}t$, $\int_x^\infty \alpha_-(t)\mathrm{d}t$ and $I_-(x)$, $I_+(x)$ are successively evaluated. Note that the integral I_- may converge rather slowly depending on the rate of decay of the potential $V(x)$ and on the size of $|z|$. One has to choose a suitable method for evaluating I_- according to the behaviour of the integrand.

6.3. **Second method.** Let us normalise the formerly introduced $u_-(x)$ so that $u_-(x)\mathrm{e}^{zx} \to 1$ as $x \to \infty$ ($d_- = 1$ in (14)). Then

$$u_-(x) = \mathrm{e}^{-zx}\gamma(x), \qquad \gamma(x) = \exp\left(\int_\infty^x \alpha_-(t)\mathrm{d}t\right). \tag{24}$$

A general solution of (10) is given by

$$f(x) = u_-(x)\left(c_1 + c_2\int_0^x \frac{\mathrm{d}t}{u_-(t)^2}\right), \tag{25}$$

where c_1, c_2 are arbitrary constants. We take $c_2 = 2z$ and look for such c_1 that $f(x) = \mathrm{e}^{zx} + o(u_-(x))$, $x \to \infty$. From (25) we then have

$$\begin{aligned} c_1 = \lim_{x\to\infty}\left(\frac{\mathrm{e}^{zx}}{u_-(x)} - 2z\int_0^x \frac{\mathrm{d}t}{u_-(t)^2}\right) = \\ = u_-(0)^{-1} + \int_{\mathbf{R}^+} \frac{\mathrm{e}^{zx}(zu_-(x) - u_-'(x)) - 2z}{u_-(x)^2}\mathrm{d}x = \\ = u_-(0)^{-1} + \int_{\mathbf{R}^+} \frac{\mathrm{e}^{2zx}(\gamma(x)(2z - \alpha_-(x)) - 2z)}{\gamma(x)^2}\mathrm{d}x. \end{aligned}$$

Everything is expressed in terms of α_- in the above formula; $u_-(0)$, $\gamma(x)$ are evaluated by means of (24). Having found c_1 we observe that $f(0) = c_1u_-(0)$, $f'(0) = c_1u_-'(0) + 2zu_-(0)^{-1}$. It remains to find the resonances from (11) as before.

The two methods described above along with the method of [2] based on complex scaling have been successfully applied to several problems to be considered in the next section. For a number of problems dealt with here (see the next section) the numerical efficiency of the two methods appears to be approximately the same. Choosing between them is a matter of convenience, although there may be situations when one of them is somewhat better than the other. We observe that the methods of this section are equivalent within the range of their consistency.

7. EXAMPLES

7.1. **Gaussian potential.** In certain cases no useful information about the resonances of the operator H can be obtained by the complex scaling method. For example if we put

$$H_gf(x) := -\Delta f(x) - \mathrm{e}^{-x^2}f(x) \tag{26}$$

acting in $L^2(\mathbf{R}^+)$ subject to Dirichlet or Neumann boundary conditions at 0, then complex scaling can only be applied for angles $\theta \le \pi/2$. However all known resonances λ of this operator have $-\pi < \arg(\lambda) < -\pi/2$, so they cannot be computed using the complex scaling technique [10].

We take the operator H_g as an example and find its resonances by means of the method of subsection 6.2. The results given in table 1

TABLE 1. Resonances for the Gaussian potential

n	λ_n
1 (D)	-0.52964412
2 (N)	$-1.23692584 - 3.48426766i$
3 (D)	$-1.33981054 - 6.70063305i$
4 (N)	$-1.45338641 - 9.95215592i$
5 (D)	$-1.59459136 - 13.14969428i$
6 (N)	$-1.69788643 - 16.29120850i$
7 (D)	$-1.75150063 - 19.43849866i$
8 (N)	$-1.80493057 - 22.61135566i$
9 (D)	$-1.87573378 - 25.77287400i$
10 (N)	$-1.93288884 - 28.91106441i$
11 (D)	$-1.96680887 - 32.05477086i$
12 (N)	$-2.00314399 - 35.21335337i$
13 (D)	$-2.05016204 - 38.36530926i$
14 (N)	$-2.13212307 - 41.49620539i$
15 (D)	$-2.11478618 - 44.64676494i$
16 (N)	$-2.14162017 - 47.79467138i$
17 (D)	$-2.16811153 - 50.85272557i$

are obtained up to the accuracy of 10^{-8}. Some of the smaller resonances of the same operator, presented very approximately in [10], are at least in a qualitative agreement with our results. The labels (D) and (N) in table 1 relate to Dirichlet and Neumann boundary conditions respectively.

Note The operator H_g is also known to have real eigenvalues. A simple variational computation shows that there is at least one eigenvalue $\lambda_0 \approx -0.335$ corresponding to the Neumann boundary condition at $x = 0$. On the other hand, it follows from [11, p. 91] that H_g cannot have more than one negative eigenvalue. This implies that the first entry in table 1 is indeed a resonance with a negligibly small imaginary part.

As well as the Gaussian potential we consider its perturbations

$$V_\varepsilon(x) = -\exp\left(\varepsilon^{-1}(1-(1+2\varepsilon x^2)^{1/2})\right),$$

for small $\varepsilon > 0$. The reason for making this rather complicated choice of perturbation is that although one cannot use complex scaling for the original potential for angles bigger than $\pi/2$, the approximating potentials allow one to use complex scaling with angles up to π, which is enough to capture the resonances of this operator. The convergence of the first two resonances of the perturbed operator to those of H_g as $\varepsilon \to 0$ is shown in table 2. The table provides a numerical confirmation of the result of theorem 10. The resonances of the perturbed and the original operator agree with the perturbation formulae of section 5. The difference is seen to be of order $O(\varepsilon)$ as expected.

TABLE 2. Perturbed resonances

ε	$\lambda_\varepsilon^{(1)} - \lambda^{(1)}$	$\lambda_\varepsilon^{(2)} - \lambda^{(2)}$
$5 \cdot 10^{-5}$	$1 \cdot 10^{-4}$	$-2 \cdot 10^{-4} + 6 \cdot 10^{-4} i$
$1 \cdot 10^{-4}$	$2 \cdot 10^{-4}$	$-3 \cdot 10^{-4} + 1.1 \cdot 10^{-3} i$
$5 \cdot 10^{-4}$	$1 \cdot 10^{-3}$	$-1.6 \cdot 10^{-3} + 5.3 \cdot 10^{-3} i$
$1 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	$-3.2 \cdot 10^{-3} + 1.06 \cdot 10^{-2} i$

7.2. **A slowly decaying modified Gaussian potential.** The operator

$$H_b f(x) := -\Delta f(x) + x^2 \mathrm{e}^{-x^2/b^2} f(x), \tag{27}$$

b being a real constant, has been studied in [2]. Here we provide more detailed information on its resonances for $b = 10$. Corollary 8 is not applicable to the operator H_b but it seems from the numerical evidence that a threshold exists. The resonances computed numerically are shown in figure 1. We used the methods of section 6 to find some of them and compared the results with those obtained in [2] by means of complex scaling. The methods agree with each other for $\operatorname{Re} z < 40$; for higher resonances complex scaling appears to be the best out of the three methods.

Theorem 6 can be applied to obtain a bound on all resonances within the sector

$$\{z : -\pi/2 < \arg(z) < 0\}.$$

For this example we have

$$a(\theta) = b^2 \sup\{s \mathrm{e}^{-s\cos(\theta)} \sin(2\theta - s\sin\theta) \,:\, s \in \mathbf{R}^+\}$$

for every $0 \le \theta < \pi/2$. This may be used to compute the envelope of the set S using the parametric formulae (6); this is compared to the actual resonances (found by complex scaling) in figure 1. Of course $a(\theta)$ may be evaluated purely numerically in more general cases. Naturally, the bounds on the resonances do not compare closely with their actual position, but it should be noted that the bounds are obtained with much less computational effort and do provide useful qualitative and quantitative information.

7.3. **The potential of Rittby et al.** We finally study the potential

$$V(x) = (x^2 - J)\mathrm{e}^{-0.1x^2} + J, \qquad J = 1.6.$$

In [9, 7, 8] one can find controversial remarks on the related resonance problem and two quite different series of resonances for the same operator. Our methods give broadly the same resonances as presented in [9]. It appears that the boundary condition at infinity taken in [7] is different from (12) as has been mentioned in [8], hence the difference between the results.

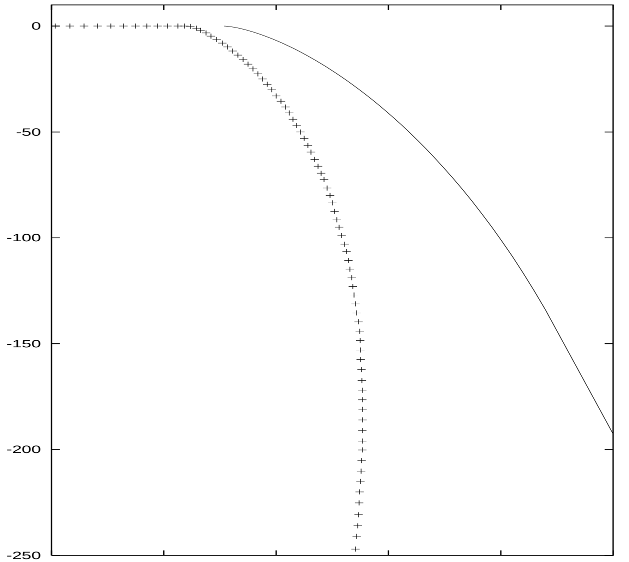

FIGURE 1. Resonances of H_b, $b = 10$, and the set S

By means of the methods of section 6 we have computed about 20 resonances, which coincide with those presented in [9] up to 4 decimal places. Computing higher resonances by either of the methods of section 6 turns out to be quite difficult, whereas the method of complex scaling still works well. Indeed, using the technique of [2] we obtain stable results which agree very well with all the resonances quoted in [9], whose method is similar. This suggests that if a potential decays fairly slowly and the complex scaling method is applicable, then it may often give more accurate results than the methods of section 6, especially for higher resonances. We have already commented that for rapidly decaying potentials like Gaussian, the methods of section 6 can be efficiently applied. It is possible to improve those methods by using an advanced technique for computing the highly oscillatory integrals involved (see the concluding remark of subsection 6.2).

Apart from the resonances found in [9, 8] we have also discovered 6 more resonances: two near each of the points $\lambda_1 = 0.69 - 7.91i$, $\lambda_2 = 1.26 - 8.51i$, $\lambda_3 = 2.08 - 11.61i$. Each pair includes an even and an odd resonance very close to one another. This closeness hinders accurate computations and is probably the reason why those resonances are missing in [9, 8]. None of our three methods allows us to locate them accurately, but there is clear evidence that they exist.

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