SYMMETRY OF BOUND AND ANTIBOUND STATES IN THE SEMICLASSICAL LIMIT

DAVID BINDEL AND MACIEJ ZWORSKI

1. Introduction and statement of the theorem

The simplest model of scattering/quantum resonances comes from considering compactly supported potentials on the real line,

$$V(x) \in \mathbb{R}, \quad |V(x)| \leq C, \quad V(x) = 0 \text{ for } |x| > L\,, \tag{1}$$

and the corresponding Schrödinger operators,

$$H_V \stackrel{\text{def}}{=} -\partial_x^2 + V(x), \tag{2}$$

on $\mathbb{R}$, or on $[0, \infty)$ with Dirichlet or Neumann boundary conditions.

The *resonances* or *scattering poles* of H_V are defined as the poles of the meromorphic continuation of the resolvent, $R_V(\lambda) = (H_V - \lambda^2)^{-1}$, from $\operatorname{Im}\lambda > 0$, to $\mathbb{C}$. Except for the poles at λ for which λ^2 are eigenvalues of H_V, $R_V(\lambda)$ is bounded on L^2 for $\operatorname{Im}\lambda > 0$. Its Schwartz kernel, that is the Green function, continues meromorphically across the continuous spectrum corresponding to $\mathbb{R}$. Its poles are the resonances of H_V.

An illustration based on the numerical codes of [4] is given in Fig.1. The poles on the positive imaginary axis correspond to the bound states of H_V, and the poles on the negative are called *antibound states*. Note that they appear to be exactly symmetric with the bound states. In this note we prove a simple theorem inspired by numerical experiments using [4]:

Theorem. *Consider the Dirichlet (or Neumann) boundary condition on* $[0, \infty)$ *and a compactly supported piecewise continuous potential* V_0, $\operatorname{supp} V_0 \subset [0, A)$. *Let* $V_1 > 0$, $B > A$, *and put*

$$V(x) = V_0(x) + \mathbb{1}_{[A,B]}(x) V_1\,.$$

Then the bound and antibound states of $H_{q^2 V}$ *with moduli greater than some fixed* $k_0 > 0$ *are symmetric modulo errors of size* e^{-cq}, $q \to \infty$.

Equivalently we can consider the semiclassical problem

$$(-(h\partial_x)^2 + V(x))u(x) = z(h)u(x)\,,$$

for which the conclusion of the theorem says that bound and antibound states with moduli greater than hk_0 are symmetric modulo exponentially small errors, $\exp(-c/h)$, as $h \to 0$.

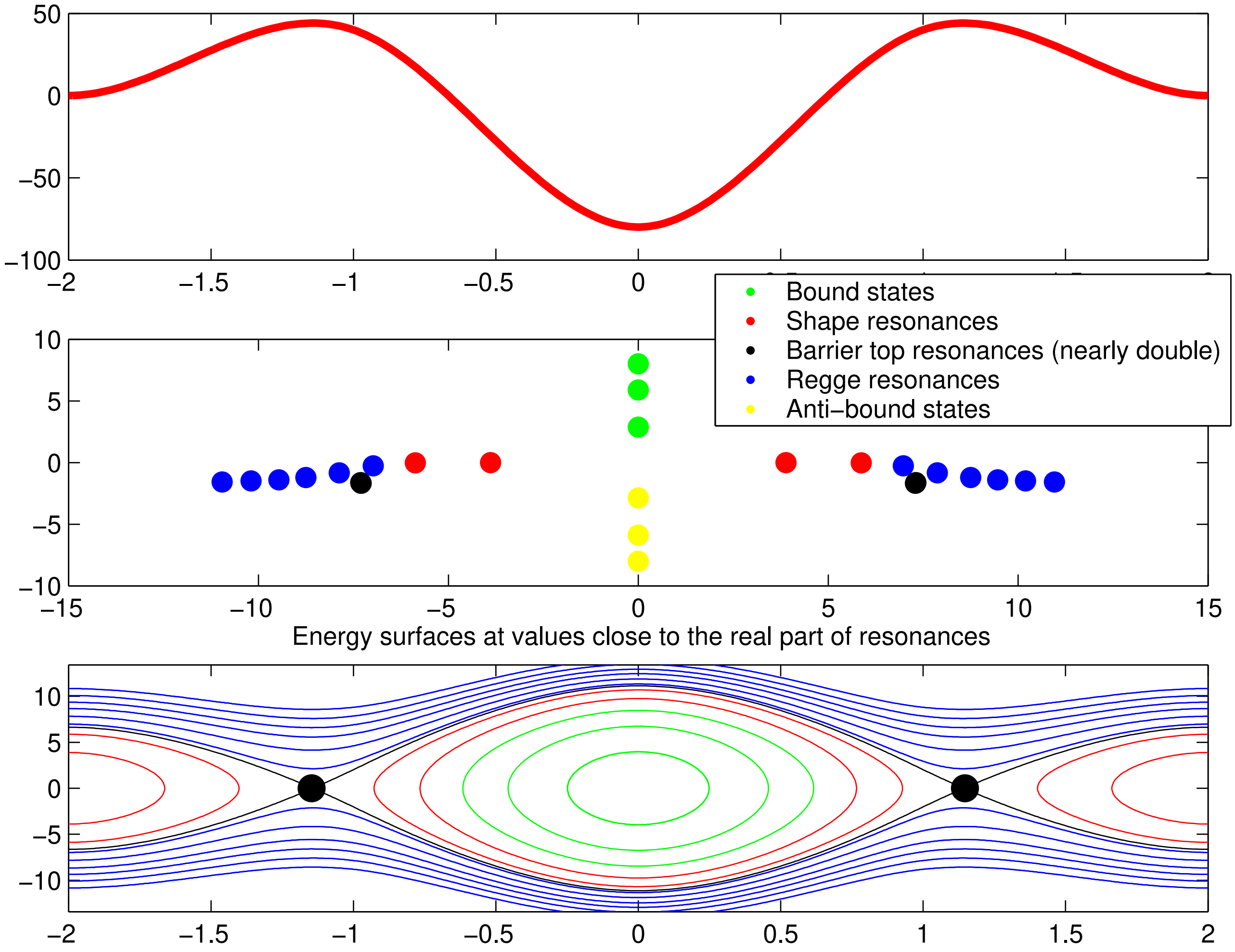

FIGURE 1. The (color coded) correspondence between classical dynamics and the distribution of resonances. The C^1 potential and its resonances are obtained using `splinepot(40*[0,1,-2,1,0],[-2,-1,0,1,2])` from [4].

We think of $\mathbb{1}_{[A,B]}(x)V_1$ as a barrier separating the potential in the interaction region, $V_0(x)$, from infinity. The same results hold on the line but the proof becomes slightly more cumbersome to write. In Fig.2 we show an example of potentials V_0, $W = V_1\mathbb{1}_{[A,B]}$, and $V = V_0 + W$. It is quite possible that using more sophisticated methods – see for instance [10] and [15] – more general barriers can be considered. Our goal here was to present a simple new result discovered by a numerical observation. It is easy to see ([17] and §2 below) that for the problem on the half line the bound and antibound states are *never* exactly symmetric. Yet, in a presence of a mild barrier, they are symmetric within numerical accuracy of a computation: the exponential convergence is indeed very rapid. This is illustrated in Fig.3: we plots of imaginary parts of bounds states and negatives of the imaginary parts of antibound states for $q^2V(x)$ as a function of q^2. The difference between the two pictures is striking. As expected the bound states are not much affected by the presence of W but the antibound states change dramatically and in the presence of a barrier become nearly symmetric (this is a curious pseudospectral effect). The high lying states of V_0 also exhibit the symmetry – experiments show that it is always so, even when there is no barrier, and it improves for more regular potentials.

The study of resonances/scattering poles in one dimension has a long tradition going back to origins of quantum mechanics, see for instance [13]. Perhaps the first study of their distribution was conducted by Regge [16]. For mathematical results in one dimension see [1],[8],[9],[11],[14],[17],[20], and many other articles. Concerning antibound states, Hitrik [9] showed (using a Ricatti equation approach which we also find useful in §2) that for positive compactly supported potentials, there are no antibound states in the semiclassical limit. That of course corresponds to our result since there are no bound states either. Simon [17] showed that for a half line problem existence of n bound states implies the existence of $n-1$ antibound states. Since the set of resonances of an even potential is the union of Dirichlet and Neumann resonances of the half line problem, this means that having n bounds states implies the existence of $2n-2$ antibound states. As can be checked using [4] this is often optimal for negative potentials but never for potentials with a barrier.

Our note is organized as follows: in §2 we give the elementary proof of the theorem and in §3 we describe the ideas behind the computation of resonances in one dimensions. The `MATLAB` codes based on that section are available at [4].

ACKNOWLEDGMENTS. The work of the second author was supported in part by a National Science Foundation grant DMS-0200732.

2. Proof of the theorem

We will prove the theorem for $A=1$ and $B=2$ – the general case is identical. We consider transfer operators for solutions of $H_{q^2V}+k^2$:

$$M_0(k):[u(0),u'(0)]\mapsto[u(1),u'(1)]$$

which depends only on V_0, q, and k, and

$$M_1(k):[u(1),u'(1)]\mapsto[u(2),u'(2)]],$$

which is completely explicit since we know V_1:

$$M_1(k)=\frac{1}{k_1}\begin{pmatrix} k_1\cosh k_1 & \sinh k_1 \\ k_1^2\sinh k_1 & k_1\cosh k_1\end{pmatrix}, \quad k_1=\sqrt{k^2+q^2V_1}>k+q/C\,. \tag{3}$$

As in the code described in §3, ik, $k>0$, is a bound state if and only if

$$M_1(k)\circ M_0(k)\,[0,1]=[\alpha,-k\alpha]\,,$$

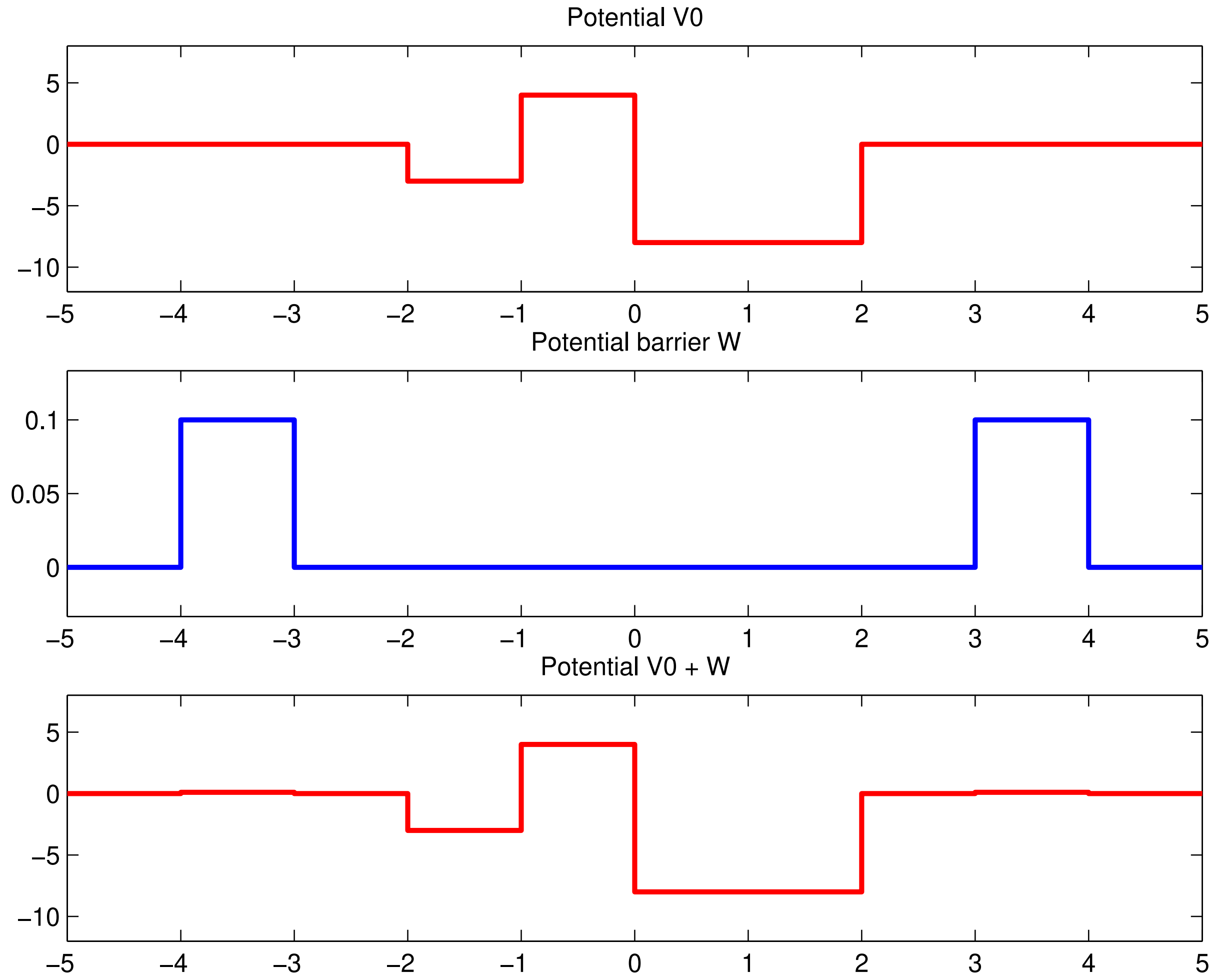

FIGURE 2. Potentials with bounds and antibound states shown in Fig.3.

for some α, and $-ik$ is an antibound state if and only if

$$M_1(k) \circ M_0(k)\,[0,1] = [\beta, k\beta]\,,$$

for some β (note that same k will never do for both, so they are *never* exactly symmetric).

The conditions for a bound $(-)$ and an antibound state $(+)$ then become (note that the left hand side depends on k and q only, and not on $\pm$):

$$\frac{u'(1)}{u(1)} = -k_1 \frac{1-\beta_\pm(k)\exp(-2k_1)}{1+\beta_\pm(k)\exp(-2k_1)}\,, \quad \beta_\pm(k) = \frac{1 \pm k/k_1}{1 \mp k/k_1}\,. \tag{4}$$

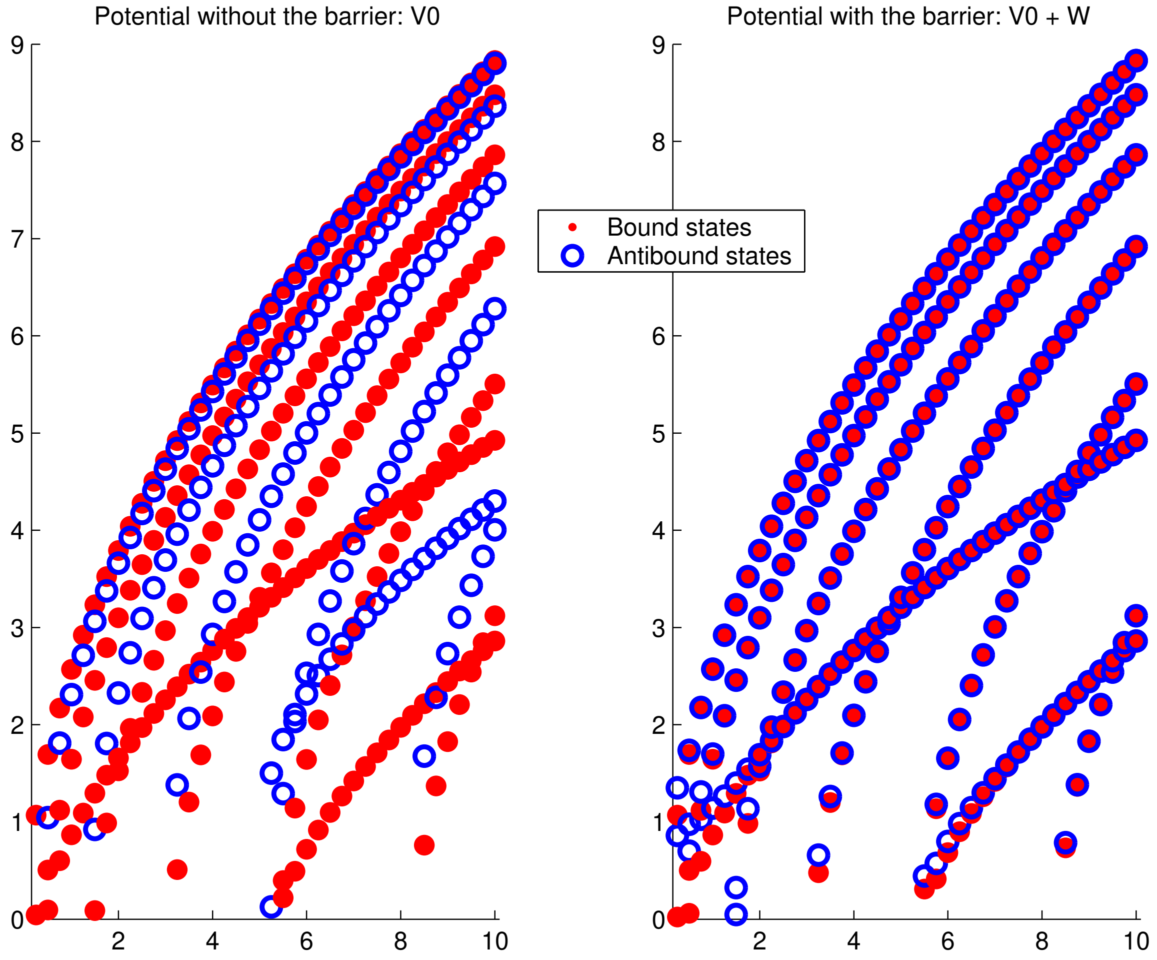

FIGURE 3. Imaginary parts, λ, of bounds states (corresponding to eigenvalues at $-\lambda^2$), and negatives of the imaginary parts of antibound states of q^2V_0, and of $q^2(V_0+W)$, as functions of q^2.

In fact, putting $v(k) \stackrel{\text{def}}{=} u'(1)/u(1)$, we use (3) to obtain the following equations for bound/antibound states:

$$\pm\frac{k}{k_1}(k_1(1+e^{-2k_1})+v(k)(1-e^{-2k_1})) = k_1(1-e^{-2k_1})+v(k)(1+e^{-2k_1}),$$

or

$$k_1\left(\pm\frac{k}{k_1}(1+e^{-2k_1})-(1-e^{-2k_1})\right) = v(k)\left(1+e^{-2k_1}\mp\frac{k}{k_1}(1-e^{-2k_1})\right),$$

from which (4) follows.

The behaviour of $v(k)$ as k varies is well known: it is monotonic between $-\infty$ and ∞ where ∞ correspond to k^2 which are Dirichlet eigenvalues of $H_{q^2 V_0}$ on $[0,1]$. But the equations for $\pm$ are the same up to exponentially small errors!

More precisely, suppose that

$$u'' = (k^2 + V(x))u\,, \quad u(0) = 0, \quad u'(0) = 1\,,$$

$u = u(x,k)$. Consider

$$v(x,k) \stackrel{\text{def}}{=} u'(x,k)/u(x,k)\,.$$

Then v satisfies the Ricatti equation

$$v' = k^2 + V - v^2\,.$$

Denote differentiation with respect to k by $\dot v$. We get the following equation for $\dot v$:

$$\dot v' = 2k - 2v\dot v\,,$$

which we can solve by the method of integrating factor. Noting that $u(x)^2 \dot v(x)|_{x=0} = 0$ (from the boundary conditions) we get

$$\dot v(x,k) = \frac{2k}{u(x,k)^2}\int_0^x u(y,k)^2 dy$$

and in particular we get an expression for the derivative of the Dirichlet to Neumann map:

$$\dot v(1,k) = \frac{2k}{u(1,k)^2}\int_0^1 u(y,k)^2 dy$$

which we can estimate from below as follows.

Since we assumed that $\operatorname{supp} V \subset [0,1)$, for some $\epsilon > 0$ we have

$$u(x,k) = Ae^{xk} + Be^{-xk}\,, \quad 1-\epsilon < x \leq 1$$

Then

$$v(1,k) = k\frac{\alpha - 1}{\alpha + 1}\,, \quad \alpha \stackrel{\text{def}}{=} \frac{A}{B}e^{2k}\,,$$

and using the same notation,

$$\begin{aligned}
\dot v(1,k) &\geq \frac{2k}{u(1,k)^2}\int_{1-\epsilon}^1 u(x,k)^2 dx \\
&= \frac{\alpha^2(1 - e^{-2k\epsilon}) + e^{2k\epsilon}(1 - e^{-2k\epsilon}) + 4\epsilon k\alpha}{(\alpha+1)^2} \qquad (5)\\
&\geq \frac{(1-\delta)(\alpha+1)^2 + \delta e^{2k\epsilon}/C}{(\alpha+1)^2} \\
&\geq 1 - \delta\,, \quad k \geq k_0(\epsilon,\delta)\,,
\end{aligned}$$

for any $\delta > 0$.

We recall that the condition (4) for being a bound (−) or an antibound (+) state was

$$v(1,k_\pm) = (k_\pm^2 + q^2 V_1)^{\frac{1}{2}}(1 + g_\pm(k_\pm, q))$$

where $g_\pm = \mathcal{O}(e^{-cq})$. Put

$$F(k) \stackrel{\text{def}}{=} \frac{v(1,k)}{(k^2 + q^2 V_1)^{\frac{1}{2}}} - 1\,,$$

so that $F(k_\pm) = g_\pm(k_\pm, q) = \mathcal{O}(e^{-cq})$. Once we show that $\dot{F}(k) \neq 0$, we will know that the roots of F are stable, and by standard theory, small perturbations to the equation lead only to small perturbations to the roots.

More precisely, we use (5) to estimate

$$\begin{aligned}\dot{F}(k) &= \frac{\dot{v}(1,k)(k^2 + q^2 V_1) - kv(1,k)}{(k^2 + q^2 V_1)^{\frac{3}{2}}} \\ &\geq \frac{(1-\delta)(\alpha+1)^2(k^2 + q^2 V_1) - k^2(\alpha^2 - 1)}{(k^2 + q^2 V_1)^{\frac{3}{2}}(\alpha+1)^2} \\ &\geq \frac{\delta}{k}\,, \quad k > k_0(\epsilon, \delta)\,,\end{aligned}$$

provided that δ is taken small enough depending on $V_1 > 0$. Hence, by the mean value theorem there exists some $0 < s < 1$, such that

$$\begin{aligned}|k_+ - k_-| &= \frac{|F(k_+) - F(k_-)|}{|\dot{F}((1-s)k_+ + sk_-)|} \\ &\leq Ce^{-2cq}((1-s)k_+ + sk_-)/\delta \\ &\leq e^{-cq}\,, \quad k_\pm > k_0\,, \quad q > q_0\,.\end{aligned}$$

Note that we used the fact that $k_\pm$ are necessarily bounded by Cq.

Replacing the explicit solutions by WKB approximations might give a more general result.

3. Numerical computation of resonances in one dimension

In this section we describe the ideas behind the codes, `squarepot.m` and `splinepot.m`, used to produce Fig.1 and 3. These `MATLAB` codes are available at [4].

If the support of V is contained in a compact interval $[-L, L]$, we can compute both resonance solutions and ordinary eigenvalues of the Schrödinger problem, $(H_V - \lambda^2)u = 0$, by writing appropriate boundary conditions at $\pm L$:

$$(6) \qquad \begin{aligned}&(H_V - \lambda^2)u = 0 && \text{for } x \in (-L, L), \\ &(\partial_x + i\lambda)u = 0 && \text{at } x = L, \\ &(\partial_x - i\lambda)u = 0 && \text{at } x = -L.\end{aligned}$$

In terms of λ, this is a *quadratic eigenvalue problem.* We can introduce a new variable $\psi = \lambda u$ to convert this problem to a linear eigenvalue problem in two fields:

$$\begin{aligned} &H_V u - \lambda\psi = 0 && \text{for } x \in (-L, L), \\ &\lambda u - \psi = 0 && \text{for } x \in [-L, L], \\ &(\partial_x - i\lambda)u = 0 && \text{at } x = L, \\ &(\partial_x + i\lambda)u = 0 && \text{at } x = -L. \end{aligned} \tag{7}$$

We now discretize the boundary and domain operators to get a finite-dimensional generalized eigenvalue problem. For small discretizations with up to a few hundred unknowns, we can solve this generalized eigenvalue problem using MATLAB's `eig` command, which uses the dense eigensolvers in LAPACK [2]. For larger discretizations, we use MATLAB's `eigs` to call ARPACK, a standard Arnoldi-based iterative eigensolver [12].

For the calculations shown in this note, we used a high-order pseudospectral collocation method to discretize the operators [19], [5]. We partition the support interval $[-L, L]$ into subintervals, and approximate u by a high-order polynomial on each subinterval. At the Chebyshev points on the interior of each subinterval, we insist that the domain differential equations be satisfied exactly, while at the junctions between neighboring intervals, we insist that the solution u and the first derivative $\partial_x u$ must both be continuous. Assuming that the potential is smooth except possibly at the endpoints of the subintervals, the collocation scheme we use is *spectrally accurate*; that is, the error asymptotically decreases faster than any algebraic function of the order of the collocation scheme. As a simple check on the accuracy of the computed eigenvalues of (7), we increase the order of the method by 50%, recompute the eigenvalues, and compare the results obtained from the coarser and the finer discretization.

We can write the analogue of (6) in higher dimensions, with a *Dirichlet-to-Neumann (DtN) map* – or some approximation to a DtN map – in place of the boundary conditions at $\pm L$. In more than one space dimension, this boundary map ceases to be a linear function of λ, and so we cannot easily convert the problem into a linear eigenvalue problem. Researchers are studying these more complicated *nonlinear eigenvalue problems* for a variety of engineering problems [3]. Many of these problems involve resonances in models of elastic, acoustic, or electromagnetic resonators with radiation losses.

For comparison, we will also discuss other methods for computing resonances. They are essential for effective codes for higher dimensional problems for which analogues of (6) are unavailable or become more complicated.

Often, resonances are computed by changing the equation so that it is no longer posed on all of $\mathbb{R}$, but instead is posed on some interval $(-M, M)$ with homogeneous Dirichlet or Neumann boundary conditions. For example, if the support of V lies strictly within the interval $(-L, L)$, we might add a *complex absorbing potential* outside of $(-L, L)$, or we might scale the coordinate system into the complex plane by the method of *perfectly* *matched layers*[1]. The change to the equation should be designed so that the modified equation mimics the behaviour of the original problem in the range $(-L, L)$.

To be more concrete, suppose that we modify the equation on the interval (L, M) so that we still have a nonsingular, second-order, ordinary differential equation in x whose coefficients depend on λ. Now we specify two linearly independent solutions $\gamma_+(x, \lambda)$ and $\gamma_-(x, \lambda)$ on (L, M) which satisfy the modified domain equation together with the initial conditions

$$\begin{aligned} \gamma_+(L, \lambda) = 1, \quad \partial_x \gamma_+(L, \lambda) = i\lambda \\ \gamma_-(L, \lambda) = 1, \quad \partial_x \gamma_-(L, \lambda) = -i\lambda. \end{aligned} \tag{8}$$

These initial conditions are consistent with the conditions for outgoing and incoming waves on $(L - \epsilon, L)$. Now suppose that $\gamma(x, \lambda)$ satisfies the differential equation on (L, M), and also the boundary condition $\gamma(M, \lambda) = 0$. Then

$$\gamma(x, \lambda) = c\,(\gamma_+(x, \lambda) + \rho\gamma_-(x, \lambda)) \tag{9}$$

where c is an arbitrary constant and

$$\rho(\lambda) \stackrel{\text{def}}{=} -\frac{\gamma_+(M, \lambda)}{\gamma_-(M, \lambda)}$$

is a constant whose amplitude reflects how well the equation on (L, M) serves to absorb outgoing waves. We can therefore convert the condition at $x = M$ to a condition at $x = L$. Subsituting (8) into (9), we have

$$\partial_x \gamma(L) - i\lambda \left(\frac{1 - \rho(\lambda)}{1 + \rho(\lambda)} \right) \gamma(L) = 0,$$

which, for regions of the complex plane where $|\rho(\lambda)|$ is small, can be treated as a perturbation of the exact outgoing wave condition at L.

In summary, by changing the Schrödinger equation outside the interval $(-L, L)$, imposing homogeneous Dirichlet boundary conditions at $\pm M$, and then transporting the conditions at $\pm M$ to conditions at $\pm L$, we arrive at the equations

$$\begin{aligned} &(H_V - \lambda^2)\hat{u} = 0 && \text{for } x \in (-L, L), \\ &(\partial_x + i\hat{\lambda})\hat{u} = 0 && \text{at } x = L, \\ &(\partial_x - i\hat{\lambda})\hat{u} = 0 && \text{at } x = -L. \end{aligned} \tag{10}$$

where

$$\hat{\lambda} \stackrel{\text{def}}{=} \lambda \left(\frac{1 - \rho(\lambda)}{1 + \rho(\lambda)} \right).$$

For values of λ where $|\rho(\lambda)| \ll 1$, (6) and (10) may be treated each as a perturbation of the other. We note that $\rho(\lambda)$ and $\beta_\pm(k) \exp(-2k_1)$ of (4) play similar rôles in the two situations. However, the smallness of $\rho(\lambda)$ is achieved through ellipticity due to the complex

[1] See [7] for a comparison of that method with the complex scaling method described, for instance, in [18]

deformation, and the smallness of $\beta_\pm(k)\exp(-2k_1)$ is due to the presence of a real barrier, $V_1 \mathbb{1}_{[0,1]}$.

The relation between outgoing wave boundary conditions and wave behaviour at the boundary of a bounded absorber is useful for applications and experiments as well as for calculations. Experiments to observe acoustic (or electromagnetic) resonances and scattering are generally conducted in *anechoic chambers*, which are lined with baffles of sound-absorbing material. These baffles prevent incoming reflected waves from interfering with the experiment. Just as one can mimic the "radiation-only" property of an infinite domain with a finite absorber, models set in infinite domains are often approximations of models over a large finite domain in which the medium through which waves propogate is slightly dissipative.

References

[1] A.A. Abramov, A. Aslanyan, and E.B. Davies, *Bounds on complex eigenvalues and resonances*, J. Phys. A **34**(2001), 57–72.

[2] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen. *LAPACK Users' Guide.* SIAM, 1999.

[3] Z. Bai and C. Yang, *From Self-Consistency to SOAR: Solving Large-Scale Nonlinear Eigenvalue Problems,* SIAM News **39**(3)(2006).

[4] D. Bindel and M. Zworski, Resonances in one dimensional: theory and computation (including `MATLAB` codes), `www.cims.nyu/~dbindel/resonant1D`

[5] J.P. Boyd, *Chebyshev and Fourier Spectral Methods.* Dover, 2001.

[6] P. Briet, J.-M. Combes, and P. Duclos, *On the location of resonances in the semi-classical limit II,* Comm. Math. Phys. **12**(1987), 201-222.

[7] K. Datchev, Computing resonances by generalized complex scaling. `http://math.berkeley.edu/~datchev/resonance3.ps`

[8] R. Froese, *Asymptotic distribution of resonances in one dimension,* J. of Diff. Equations, **137**(2), (1997), 251–272.

[9] M. Hitrik, *Bounds on scattering poles in one dimension,* Comm. Math. Phys. **208**(1999), 381–411.

[10] S. Fujiye and T. Ramond, *Matrice de scattering et résonances associées à une orbite hétérocline,* Ann. IHP, Physiqie Théorique, **69**(1998), 31-82.

[11] E. Korotyaev, *Inverse resonance scattering on the real line,* Inverse Problems **21**(2005), 325–341.

[12] R.B. Lehoucq, D. Sorensen, and C. Yang, *ARPACK User's Guide: Solution of Large-Scale Eigenvalue Problems with Implicitly Restarted Arnoldi Methods.* `http://www.caam.rice.edu/software/ARPACK/UG/ug.html` SIAM, 1998.

[13] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory,* Third Edition, Elsevier, 1977.

[14] L. Nedelec, *Asymptotics of resonances for matrix valued Schrödinger operators,* `math.SP/0509391`.

[15] T. Ramond, *Semiclassical study of quantum scattering on the line,* Comm. Math. Phys. **177**(1996), 221–254.

[16] T. Regge, *Analytic properties of the scattering matrix,* Nuovo Cimento, **10**(1958), 671-679.

[17] B. Simon, *Resonances in one dimension and Fredholm determinants,* J. Funct. Anal. **178**(2000), 396–420.

[18] S.H. Tang and M. Zworski, *Potential scattering on the real line,* `http://math.berkeley.edu/~zworski/tz1.pdf`

[19] L.N. Trefethen, *Spectral Methods in MATLAB,* SIAM, 2000.
[20] M. Zworski, *Distribution of poles for scattering on the real line,* J. Funct. Anal. **73**(1987), 277-296.

Department of Mathematics, Courant Institute of Mathematical Sciences, New York University, New York, NY 10012

E-mail address: dbindel@cims.nyu.edu

Mathematics Department, University of California, Evans Hall, Berkeley, CA 94720, USA

E-mail address: zworski@math.berkeley.edu