Bounds and Error Estimates for Resonance Problems

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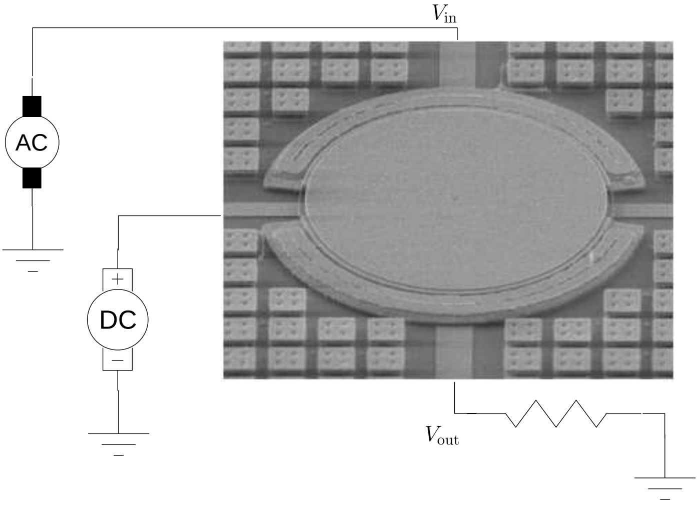
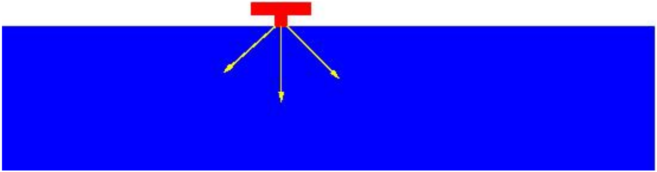
Why Resonances?



Why Resonances?



- Dominant energy loss from radiation into substrate.
- No L^2 eigenfunction associated with vibrational mode.
- This is a resonance computation!

The Big Picture

Problem: Good methods and theory for finite-dimensional eigenvalue problems and PDEs on compact domains. Can we extend to resonances for PDEs on unbounded domains?

The approach:

- Resonance computations as *nonlinear* eigenproblems.
- Backward error analysis via perturbations.
- Bounds via generalized spectral inclusion regions.

Simple 1D Problem

Consider 1D Schrödinger (V nice, $\text{supp}(V) \subset [a, b]$):

$$H\psi = \left(-\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi.$$

- H self-adjoint with discrete spectrum on $E < 0$, continuous spectrum on $E \geq 0$.
- Continuous spectrum is a branch cut for the resolvent. (Think $\chi(H - E)^{-1}\chi$, χ a smooth cutoff, $\chi([a, b]) = 1$. One moral analogue of a spectral Schur complement.)
- Second-sheet poles of the resolvent are *resonances*. Correspond to trapping, quasi-stable states.

Simple 1D Problem

Consider 1D Schrödinger:

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi.$$

How do we:

1. Quickly compute resonances (nice enough V)?
2. Make sure the computations are correct?

Simple 1D Problem

Consider 1D Schrödinger:

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi.$$

If $\mathrm{supp}(V) \subset [a, b]$, write

$$\begin{aligned}\left(-\frac{d^2}{dx^2} + V(x) - k^2\right)\psi &= 0, x \in (a, b)\\ \left(\frac{d}{dx} - ik\right)\psi &= 0, x = b\\ \left(\frac{d}{dx} + ik\right)\psi &= 0, x = a\end{aligned}$$

$\Im k \geq 0$ for eigenvalues, $\Im k < 0$ for resonances.

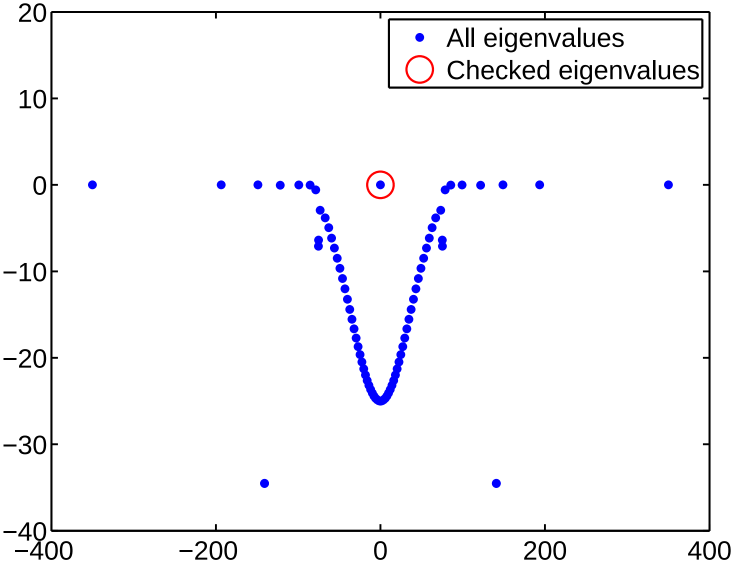
Pseudospectral Discretization

Sample ψ at Chebyshev nodes and approximate $d\psi/dx$ by differentiating the interpolant:

$$\left(-D^2 + V(x) - k^2\right)\psi = 0, x \in (a, b)$$
$$(D - ik)\,\psi = 0, x = b$$
$$(D + ik)\,\psi = 0, x = a$$

Now linearize (introduce auxiliary variable $\phi = k\psi$) to get an ordinary generalized eigenvalue problem.

Is it that easy?



Backward Error Analysis

If $\hat{\psi}$ is a numerical solution, there is some $\hat{V}$ s.t.

$$\left(-\frac{d^2}{dx^2} + \hat{V}(x) - k^2\right)\hat{\psi} = 0, x \in (a, b)$$

First-order sensitivity to changes in $\hat{V}$ is

$$\begin{aligned}\delta k &= \frac{\int_a^b \hat{\psi}(\delta V)\hat{\psi}}{2k\int_a^b \hat{\psi}^2 + i(\hat{\psi}^2(a) + \hat{\psi}^2(b))} \\ &= \frac{\int_a^b \hat{\psi}(H_V - k^2)\hat{\psi}}{2k\int_a^b \hat{\psi}^2 + i(\hat{\psi}^2(a) + \hat{\psi}^2(b))}.\end{aligned}$$

Compute $\hat{V}$ by evaluating residual for approximate $\hat{\psi}$ on a fine mesh.

More General Picture

Consider Schrödinger with compactly supported V in R^d. On resolvent set,

$$\begin{aligned} (H_V - E)\psi &= f \text{ on } \Omega \\ \frac{\partial \psi}{\partial n} - B(E)\psi &= 0 \text{ on } \Gamma \end{aligned}$$

where $B(E)$ is the Dirichlet-to-Neumann map on $\partial\Omega$
Admits a variational formulation:

$$\begin{aligned} I(\psi) &= \frac{1}{2}\int_\Omega \left((\nabla\psi)^T(\nabla\psi) + \psi(V-E)\psi\right)\, d\Omega + \\ & \frac{1}{2}\int_\Gamma \psi B(E)\psi \, d\Gamma - \int_\Omega \psi f \, d\Omega. \end{aligned}$$

Rayleigh Quotient Analogue

Now define a residual for an approximate eigenpair:

$$r(\psi, E) = \int_\Omega \Big((\nabla\psi)^T (\nabla\psi) + \psi(V - E)\psi \Big) + \int_\Gamma \psi B(E)\psi.$$

Take variations and use symmetry of B:

$$\begin{aligned} \delta r(\psi, E) &= 2\int_\Omega \delta\psi \left[(-\Delta + V - E)\psi\right] + \\ & \quad 2\int_\Gamma \delta\psi \left[\frac{\partial\psi}{\partial n} - B(E)\psi\right] + \\ & \quad \delta E \left[\int_\Omega \psi^2 - \int_\Gamma \psi B'(E)\psi\right] \end{aligned}$$

Rayleigh Quotient Analogue

We now implicitly define a differentiable function $\tilde{E}(\psi)$ in the neighborhood of an eigenpair (ψ, E_*), with $r(\psi, E(\psi)) = 0$ and $E(\psi) = E_*$. Such a function should exist if

$$\int_\Omega \psi^2 - \int_\Gamma \psi B'(E)\psi \neq 0$$

Stationary precisely when (ψ, E) an eigenpair.

Sensitivity

Now assume δV a compactly-supported perturbation, and look at effect of δV on Rayleigh quotient analogue. Gives that isolated eigenvalues change like

$$\delta E = \frac{\int_\Omega \delta V \psi^2}{\int_\Omega \psi^2 - \int_\Gamma \psi B'(E) \psi}$$

Can also write in terms of a residual for ψ as a solution for the potential $V + \delta V$:

$$\delta E = \frac{\int_\Omega \psi(-\Delta + (V + \delta V) - E)\psi}{\int_\Omega \psi^2 - \int_\Gamma \psi B'(E) \psi}.$$

Approximating NEPs

Can be hard to find all nonlinear eigenvalues in a region! Want:

- Approximating problem that is easier to analyze (e.g. approximate DtN by perfectly matched layer or other absorbing boundary)
- Theory to relate the spectrum for the original NEP and the approximation.

Example: Lattice Schrödinger

Consider the discrete analogue to Schrödinger's equation:

$$H\psi = (-T + V)\psi = E\psi$$

where

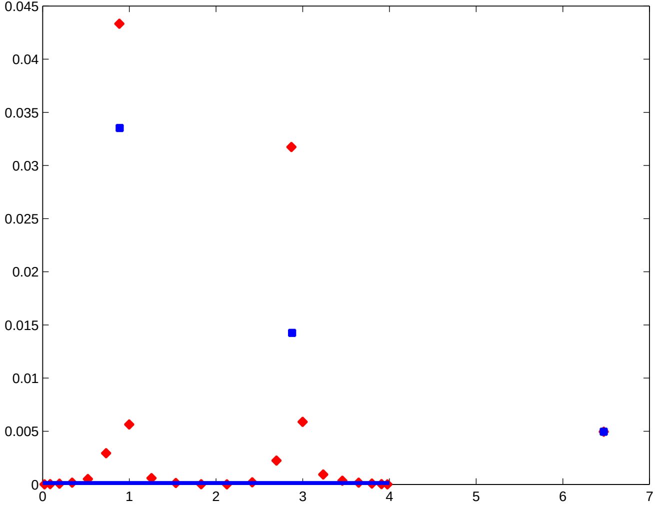
$$(H\psi)_k = -\psi_{k-1} + 2\psi_k - \psi_{k+1} + V_k\psi_k.$$

Assume $V_k = 0$ for $k \leq 0$ and $k \geq L$. May be complex.

Want to relate the spectrum for two variants:

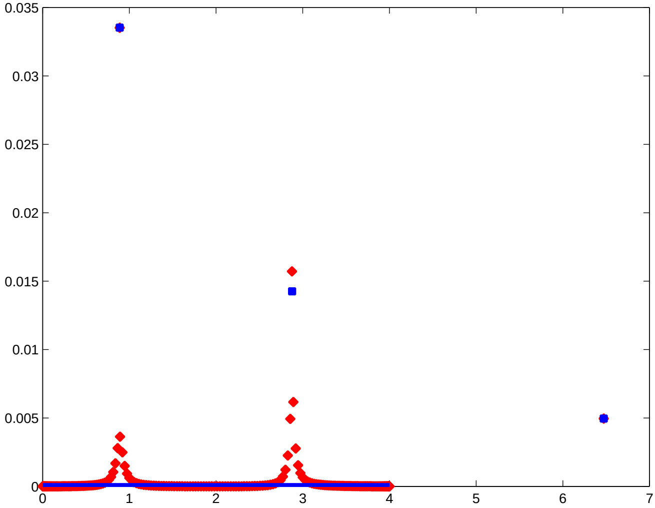
1. Non-negative integers: $\psi_0 = 0$ and $\psi \in l^2$
2. Bounded: $\psi_k = 0$ for $k = 0$ and $k \geq L + N$.

Example: Lattice Schrödinger



For $V_2 = 0.1i$ and $V_3 = 4$, $N = 20$.

Example: Lattice Schrödinger



For $V_2 = 0.1i$ and $V_3 = 4$, $N = 200$.

Spectral Schur complement

Write H in either case as

$$H = \begin{bmatrix} -T_{11} + V_{11} & -e_L e_1^T \\ -e_L e_1^T & -T_{22} \end{bmatrix}$$

Then $\Lambda(H) \cap \Lambda(-T_{22})^c = \Lambda(S)$, where

$$S(z) = (-T_{11} + V_{11}) - zI - \left(e_1^T (-T_{22} - zI)^{-1} e_1 \right) e_L e_L^T$$

Write $S^{(N)}(z)$ and $S^{(\infty)}(z)$ for bounded and unbounded cases.

Spectral Schur complement

For $z \notin [0,4]$, choose $\xi^2 - (2-z)\xi + 1 = 0$, $|\xi| < 1$. Then

$$\begin{aligned} S^{(\infty)}(z) &= (-T_{11} + V_{11}) - zI - \xi e_L e_L^T \\ S^{(N)}(z) &= (-T_{11} + V_{11}) - zI - \xi \left(\frac{1 - \xi^{2N}}{1 - \xi^{2(N+1)}} \right) e_L e_L^T \end{aligned}$$

Convenient to write $z = 2 - \xi - \xi^{-1}$, use ξ as primary variable.

How do we compare $S^{(\infty)}(z)$ and $S^{(N)}(z)$?

Counting eigenvalues

If A nonsingular on Γ, analytic inside, count eigs inside by

$$\begin{aligned} W_\Gamma(\det(A)) &= \frac{1}{2\pi i} \int_\Gamma \frac{d}{dz} \ln\det(A(z))\, dz \\ &= \operatorname{tr}\left(\frac{1}{2\pi i} \int_\Gamma A(z)^{-1} A'(z)\, dz \right) \end{aligned}$$

Suppose E also analytic inside Γ. By continuity,

$$W_\Gamma(\det(A)) = W_\Gamma(\det(A + sE))$$

for s in neighborhood of 0 such that $A + sE$ remains nonsingular on Γ.

Idea

Winding number counts give continuity of eigenvalues $\implies$
Should consider eigenvalues of $A + sE$ for $0 \leq s \leq 1$:

Analyticity of A and E +
Matrix nonsingularity test for $A + sE$ =

Inclusion region for $\Lambda(A + E)$ +
Eigenvalue counts for connected components of region

Example: Matrix Rouché

$\|A^{-1}(z)E(z)\| < 1$ on $\Gamma \implies$ same eigenvalue count in Γ

Proof:
$\|A^{-1}(z)E(z)\| < 1 \implies A(z) + sE(z)$ invertible for $0 \leq s \leq 1$.

(Gohberg and Sigal proved a more general version in 1971.)

Example: Nonlinear Gershgorin

Define

$$G_i = \left\{ z : |a_{ii}(z)| < \sum_{j \neq i} |a_{ij}(z)| \right\}$$

Then

1. $\Lambda(A) \subset \cup_i G_i$
2. Connected component $\cup_{i=1}^m G_i$ contains m eigs (if bounded and disjoint from $\partial\Omega$)

Proof: Write $A = D + F$ where $D = \mathrm{diag}(A)$.
$D + sF$ is diagonally dominant (so invertible) off $\cup_i G_i$.

Example: Pseudospectral Containment

Define $D = \{z : \|E(z)\| < \epsilon\}$. Then

1. $\Lambda(A + E) \subset \Lambda_\epsilon(A) \cup D^C$
2. A bounded component of $\Lambda_\epsilon(A)$ strictly inside D contains the same number of eigs of A and $A + E$.

Error Bounds for Discrete Schrödinger

Find $\|S^{(\infty)} - S^{(N)}\| \leq \epsilon$ if

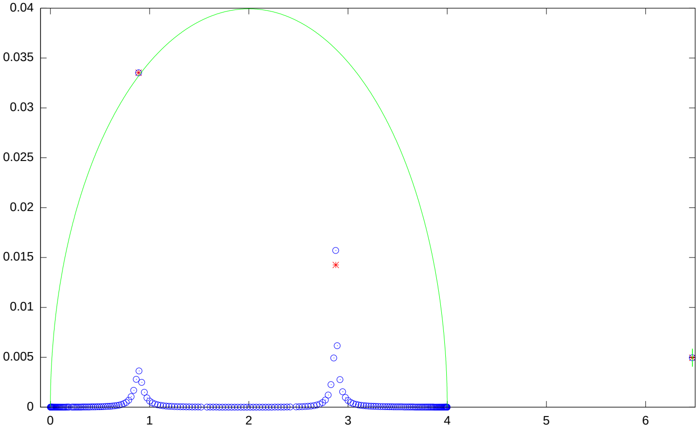
$$|\xi| < \left(1 + \frac{\log(3\epsilon^{-1})}{2N+1}\right)^{-1} = 1 - O\left(\frac{\log(\epsilon^{-1})}{N}\right).$$

Therefore, eigenvalues in bounded case (in ξ plane) either

1. Are within $O(\log(\epsilon^{-1})/N)$ of circle (continuous spectrum)
2. Are in $\Lambda_\epsilon(S^{(\infty)})$.

Get exponential convergence to discrete spectrum, linear convergence to continuous spectrum.

Error Bounds for Discrete Schrödinger



Eigenvalues from $N = 200$ plus bound with $\epsilon = 10^{-3}$.
Actual error in eigenvalue near one: `1.28e-5`.
Error bound: `1.55e-5`

Conclusions

1. Can reduce resonance computations and eigenproblems (from infinite to finite, from big to smaller) via spectral Schur complementation.
2. Can apply backward error analysis to computed eigenvalues for resulting NEPs.
3. Can relate eigenvalues of desired NEP and an approximation in order to get bounds on spectrum in part of the complex plane.