

# Bounds and Error Estimates for Nonlinear Eigenvalue Problems

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# Outline

Resonances via nonlinear eigenproblems

Sensitivity and backward error analysis

Resonances via Perfectly Matched Layers

Perturbation bounds

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# 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  $\chi(H - E)^{-1}\chi$ ,  $\chi$  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  $\text{supp}(V) \subset [a, b]$ , write

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

$$\left(\frac{d}{dx} - ik\right)\psi = 0, x = b$$

$$\left(\frac{d}{dx} + ik\right)\psi = 0, x = a$$

$E = k^2$ ,  $\text{Im } k \geq 0$  for eigenvalues,  $\text{Im } k < 0$  for resonances.

# Pseudospectral Discretization

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

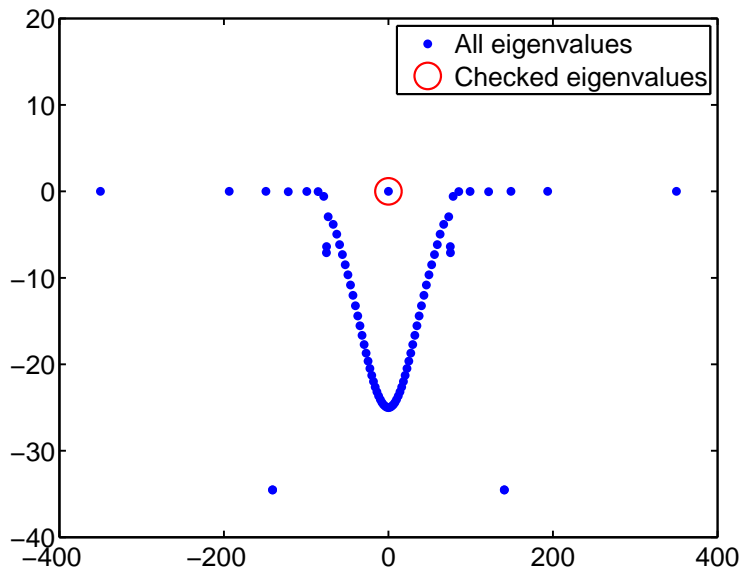
$$\left(-D^2 + V(x) - k^2\right) \psi = 0, x \in (a, b)$$

$$(D - ik) \psi = 0, x = b$$

$$(D + ik) \psi = 0, x = a$$

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

# Is it that easy?



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# Backward Error Analysis

1. If  $(\hat{\psi}, \hat{E})$  is a numerical solution with above scheme, then there is some  $\hat{V}$  s.t. for  $x \in (a, b)$ ,

$$(H_{\hat{V}} - \hat{E})\hat{\psi} = \left( -\frac{d^2}{dx^2} + \hat{V}(x) - \hat{E} \right) \hat{\psi} = 0$$

together with corresponding radiation conditions.

2. Estimate  $\hat{V}$  explicitly by remapping residual to finer mesh
3. Original problem is a perturbation of computed problem.
4. Use first-order perturbation theory to correct  $\hat{E}$ .  
Useful to take a *variational* approach.

## More General Picture

Consider Schrödinger with compactly supported  $V$  in  $R^d$ .  
For  $E$  in resolvent set on appropriate Riemann surface, seek

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

where  $B(E)$  is the Dirichlet-to-Neumann map on  $\partial\Omega$ .  
Solutions are stationary points for

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

# Variational Formulation

Check variational formulation:

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

Use symmetry of form (note  $\int_{\Gamma} \phi B(E) \psi = \int_{\Gamma} \psi B(E) \phi$ ) + integration by parts:

$$\delta I(\psi) = \int_{\Omega} \delta \psi (-\Delta \psi + (V - E) \psi - f) d\Omega + \int_{\Gamma} \delta \psi \left( \frac{\partial \psi}{\partial n} - B(E) \right) \psi d\Gamma.$$

# Rayleigh Quotient Analogue

Now define a residual for an approximate eigenpair:

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

Take variations and use symmetry of  $B$ :

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

For an eigenpair or resonance,  $r(\psi, E) = 0$  and  $\delta r(\psi, E) = 0$ .

# Rayleigh Quotient Analogue

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

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

Stationary precisely when  $(\psi, E)$  an eigenpair.

# Sensitivity

Now assume  $\delta V$  a compactly-supported perturbation, and look at effect of  $\delta V$  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  $\psi$  as a solution for the potential  $V + \delta V$ :

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

# Backward Error Analysis Revisited

1. Compute approximate solution  $(\hat{\psi}, \hat{E})$ .
2. Map  $\hat{\psi}$  to high-resolution quadrature grid to evaluate

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

3. If  $\delta E$  large, discard  $\hat{E}$  as spurious; otherwise, accept  $E \approx \hat{E} + \delta E$ .

# Some Computational Issues

In general, using the domain equation + DtN map to find resonances is problematic because:

1. The DtN map is nonlocal, expensive to work with computationally.
2. The Green's function (and hence the DtN map) are hard to compute for some problems I care about (e.g. elastic half space problems).
3. Nonlinear eigenvalue problems are trickier than linear problems to solve.

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Sensitivity and backward error analysis

**Resonances via Perfectly Matched Layers**

Perturbation bounds

# Perfectly Matched Layers

For scattering computations / resonance computations, need an outgoing BC. We use *perfectly matched layers*:

- ▶ Complex coordinate transformation
- ▶ Generates a “perfectly matched” absorbing layer
- ▶ Rotates the continuous spectrum to reveal resonances
- ▶ Idea works with general linear wave equations
  - ▶ Electromagnetics (Bereng er, 1994)
  - ▶ Quantum mechanics – *exterior complex scaling* (Simon, 1979 – originally used to *define* resonances)
  - ▶ Elasticity in standard finite element framework (Basu and Chopra, 2003)

# Model Problem

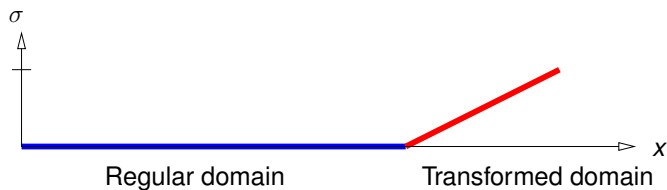
- ▶ Domain:  $x \in [0, \infty)$
- ▶ Frequency-domain equation:

$$\frac{d^2 \hat{u}}{dx^2} + k^2 \hat{u} = 0$$

- ▶ Solution:

$$\hat{u} = c_{\text{out}} e^{-ikx} + c_{\text{in}} e^{ikx}$$

# Model with Perfectly Matched Layer

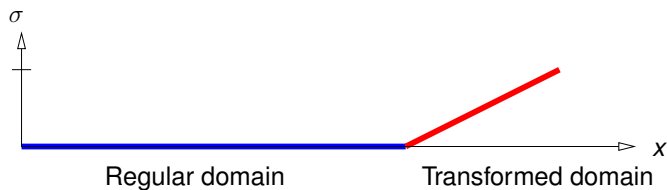


$$\frac{d\tilde{x}}{dx} = \lambda(x) \text{ where } \lambda(s) = 1 - i\sigma(s)$$

$$\frac{d^2\hat{u}}{d\tilde{x}^2} + k^2\hat{u} = 0$$

$$\hat{u} = c_{\text{out}}e^{-ik\tilde{x}} + c_{\text{in}}e^{ik\tilde{x}}$$

# Model with Perfectly Matched Layer



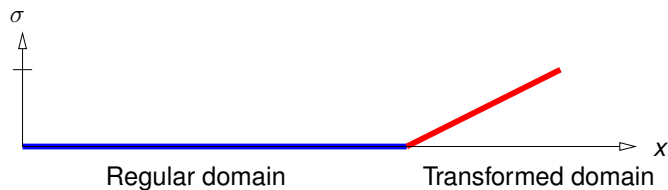
$$\frac{d\tilde{x}}{dx} = \lambda(x) \text{ where } \lambda(s) = 1 - i\sigma(s),$$

$$\frac{1}{\lambda} \frac{d}{dx} \left( \frac{1}{\lambda} \frac{d\hat{u}}{d\tilde{x}} \right) + k^2 \hat{u} = 0$$

$$\hat{u} = c_{\text{out}} e^{-ikx - k\Sigma(x)} + c_{\text{in}} e^{ikx + k\Sigma(x)}$$

$$\Sigma(x) = \int_0^x \sigma(s) ds$$

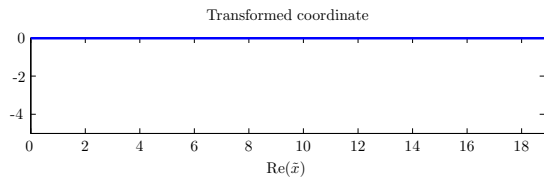
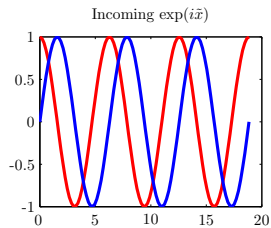
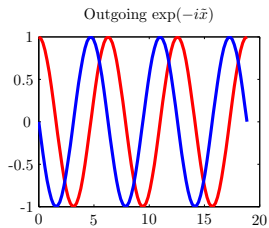
# Model with Perfectly Matched Layer



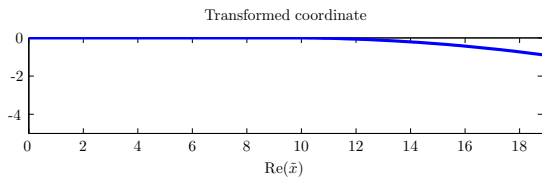
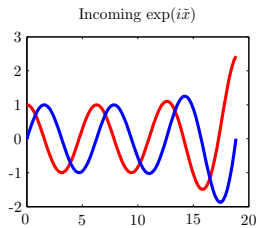
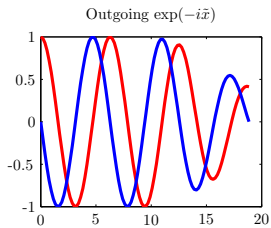
If solution clamped at  $x = L$  then

$$\frac{c_{\text{in}}}{c_{\text{out}}} = O(e^{-k\gamma}) \text{ where } \gamma = \Sigma(L) = \int_0^L \sigma(s) ds$$

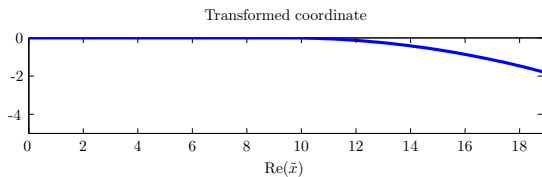
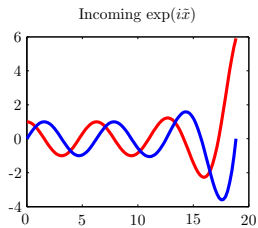
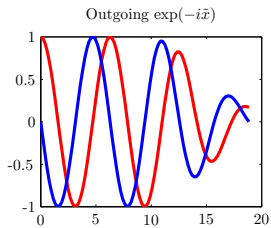
# Model Problem Illustrated



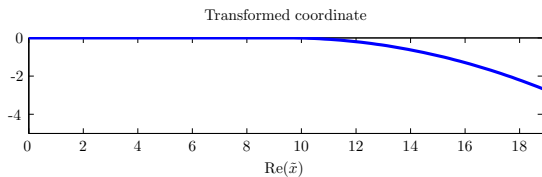
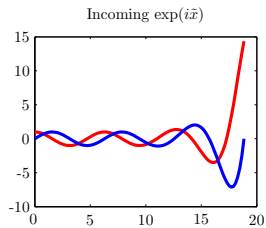
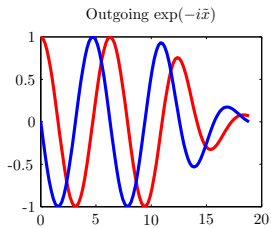
# Model Problem Illustrated



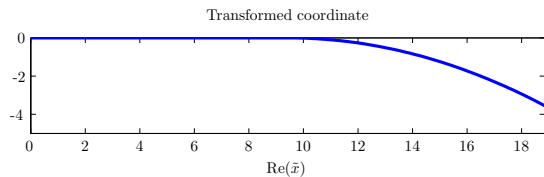
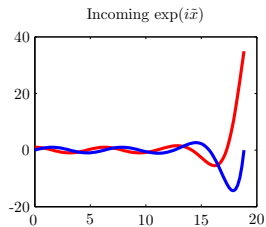
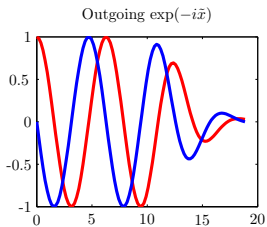
# Model Problem Illustrated



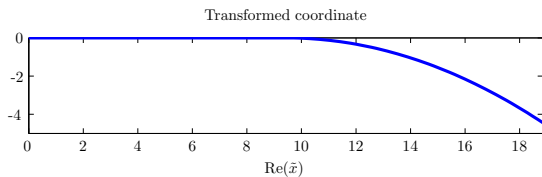
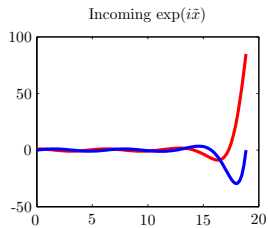
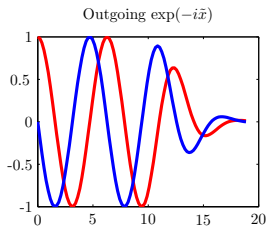
# Model Problem Illustrated



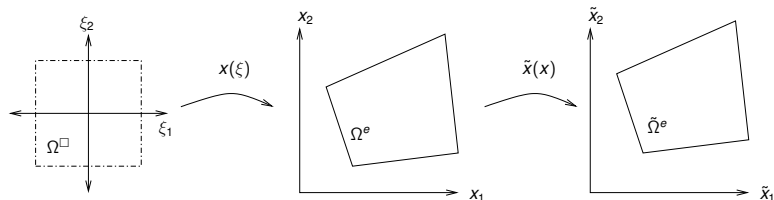
# Model Problem Illustrated



# Model Problem Illustrated



# Finite/Spectral Element Implementation



- Combine PML and isoparametric mappings

$$\mathbf{k}^e = \int_{\Omega^\square} \tilde{\mathbf{B}}^T \mathbf{D} \tilde{\mathbf{B}} \tilde{J} d\Omega^\square$$
$$\mathbf{m}^e = \int_{\Omega^\square} \rho \mathbf{N}^T \mathbf{N} \tilde{J} d\Omega^\square$$

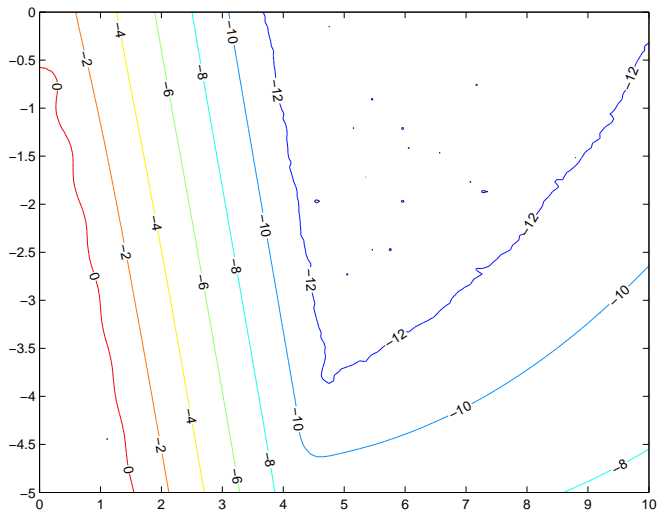
- Matrices are *complex symmetric*

# DtN Approximation in PML

- ▶ Earlier (DtN) form - Neumann form = DtN term  $\int_{\Gamma} \psi \mathbf{B} \psi$ .
- ▶ Eliminate PML dofs - Neumann form  $\approx$  DtN term
- ▶ Approximation is rational in  $k$ , good locally
- ▶ Would like to understand how good approximation to DtN + some form of stability leads to error bounds.

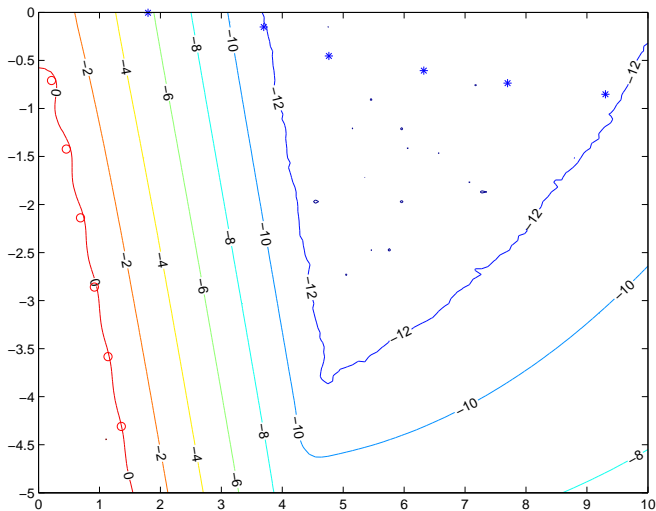
# DtN Approximation in PML

$\log_{10} |B(k)_{PML} - B(k)|$  on circle of radius 3 in  $\mathbb{R}^2$ .  
Order 30 spectral elements, PML goes [3, 4].



# DtN Approximation in PML

Axisymmetric resonances for ring barrier for  $r \in [1, 2]$ .  
Stars for small residual; circles for spurious resonance.



## Relation of PML to DtN Approach

- ▶ Numerically eliminate variables in PML  $\implies$  local (in  $k$  or  $E$ ) rational approximation to DtN-like condition.
- ▶ Could also form explicit Padé approximation.
- ▶ Approximation is local in  $k$  – where can we guarantee (for example) that we have approximated all resonances?

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# General NEP Picture

$A : \mathbb{C} \rightarrow \mathbb{C}^{n \times n}$  analytic in  $\Omega$

$$\Lambda(A) := \{z \in \mathbb{C} : A(z) \text{ singular}\}$$

$$\Lambda_\epsilon(A) := \{z \in \mathbb{C} : \|A(z)^{-1}\| \geq \epsilon^{-1}\}$$

- ▶ Resonance calculation with DtN map or with eliminated PML as an example.
- ▶  $\Lambda(A)$  and  $\Lambda_\epsilon(A)$  describe asymptotics, transients of some linear differential or difference equation.
- ▶ Lots of function theoretic proofs from analyzing ordinary eigenvalue problems carry over without change.

# Counting Eigenvalues

If  $A$  nonsingular on  $\Gamma$ , 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  $\Gamma$ . By continuity,

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

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

# Function Theoretic Perturbation Recipe

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  $\Gamma$

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  $D = \text{diag}(A)$ .

$D + sF$  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  $A + E$ .

# Application: Lattice Schrödinger

Consider the discrete analogue to Schrödinger's equation:

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

where

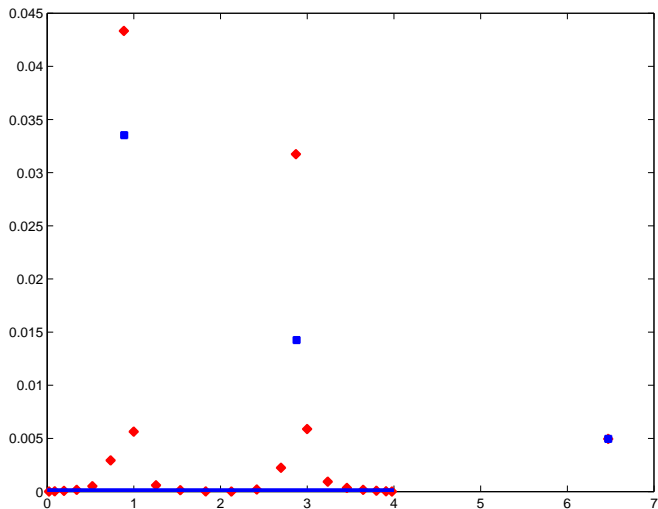
$$(H\psi)_k = -\psi_{k-1} + 2\psi_k - \psi_{k+1} + V_k\psi_k.$$

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

Want to relate the spectrum for two variants:

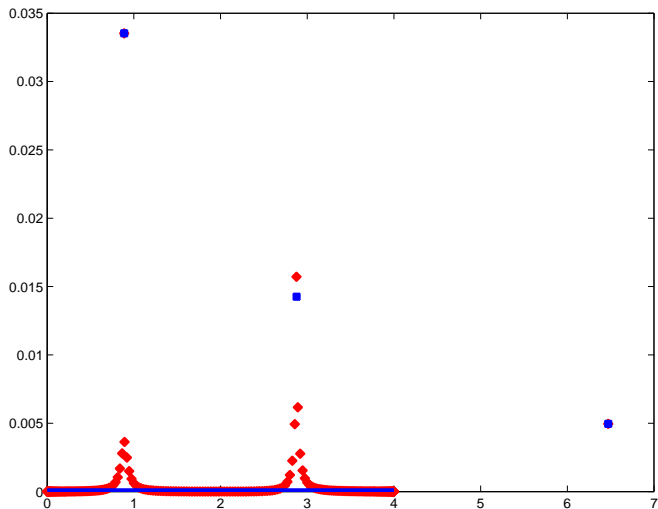
1. Non-negative integers:  $\psi_0 = 0$  and  $\psi \in \ell^2$
2. Bounded:  $\psi_k = 0$  for  $k = 0$  and  $k \geq L + N$ .

# Application: Lattice Schrödinger



For  $V_1 = 0.1i$  and  $V_2 = 4$ ,  $N = 20$ .

# Application: Lattice Schrödinger



For  $V_1 = 0.1i$  and  $V_2 = 4$ ,  $N = 200$ .

# 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

$$S^{(\infty)}(z) = (-T_{11} + V_{11}) - zI - \xi e_L e_L^T$$

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

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

# Error Bounds

Find  $\|\mathcal{S}^{(\infty)} - \mathcal{S}^{(N)}\| \leq \epsilon$  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  $\xi$  plane) either

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

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

# Error Estimate

If  $S^{(\infty)}$  has an isolated eigenvalue at  $\gamma$ , then  $S^{(N)}$  asymptotically has eigenvalues  $\gamma^{(N)} \rightarrow \gamma$  with

$$\gamma^{(N)} - \gamma = \gamma^{2N} \frac{w^* e_L e_L^T v_L}{(1 - \gamma^2) w^* v - w^* e_L e_L^T v} + O(\gamma^{2N+1})$$

where  $S^{(\infty)}(\gamma)v = 0$  and  $w^* S^{(\infty)}(\gamma) = 0$ .

# Similar Applications

- ▶ Linear stability analysis for traveling waves.
- ▶ Bounds on distance to instability via subspace projections.
- ▶ Estimates of damping in MEMS resonators.

# Conclusions

- ▶ Can write eigenvalue and resonance problems via NEP
- ▶ Variational characterization gives easy first-order perturbation theory
- ▶ For analytic NEPs, also get analogues to standard perturbation bounds (Rouché, Gerschgorin, pseudospectral)
- ▶ Get interesting problems via approximation of spectral Schur complements