Resonances:
Interpretation, Computation, and Perturbation

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Thanks, Pete!
The quantum corral
“Particle in a box” model

Schrödinger equation

\[ H\psi = (-\nabla^2 + V)\psi = E\psi \]

where

\[ V(r) = \begin{cases} 
0, & r < 1 \\
\infty, & r \geq 1 
\end{cases} \]

Result: eigenmodes of Laplace with Dirichlet BC.
Eigenfunctions at the quantum corral
A more realistic model?

Corral really looks like a *finite* potential

\[ V(r) = \begin{cases} 
V_0, & R_1 < r < R_2 \\
0, & \text{otherwise}
\end{cases} \]

Does anything change?
Electrons unbound

For a finite barrier, electrons can escape!
Not a *bound state* (conventional eigenmode).
Spectra and scattering

For compactly supported $V$, spectrum consists of

- Possible discrete spectrum (*bound states*) in $(-\infty, 0)$
- Continuous spectrum (*scattering states*) in $[0, \infty)$

We’re interested in the latter.
Resonances and scattering

For $\text{supp}(V) \subset \Omega$, consider a scattering experiment:

$$(H - k^2)\psi = f \text{ on } \Omega$$

$$(\partial_n - B(k))\psi = 0 \text{ on } \partial\Omega$$

A measurement $\phi(k) = w^*\psi$ shows a resonance peaks. Associate with a resonance pole $k^* \in \mathbb{C}$ (Breit-Wigner):

$$\phi(k) \approx C(k - k^*)^{-1}.$$
Resonances and scattering

Consider a scattering measurement $\phi(k)$

- Morally looks like $\phi = w^*(H - E)^{-1}f$?
- $w^*(H - E)^{-1}f$ is well-defined off spectrum of $H$
- Continuous spectrum of $H$ is a branch cut for $\phi$
- Resonance poles are on a second sheet of definition for $\phi$
- Resonance “wave functions” blow up exponentially (not $L^2$)
Resonances and transients

A thousand valleys’ rustling pines resound.  
My heart was cleansed, as if in flowing water.  
In bells of frost I heard the resonance die.  

– Li Bai (interpreted by Vikram Seth)
Resonances and transients

Potential

Pole locations
Resonances and transients
## Eigenvalues and resonances

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Computing resonances

Simplest method: extract resonances from $\phi(k)$

- This is the (modified) *Prony* method
- Has been used experimentally and computationally (e.g. Wei-Majda-Strauss, JCP 1988 – modified Prony applied to time-domain simulations)

There are better ways.
A nonlinear eigenproblem

Can also define resonances via a NEP:

\[(H - k^2)\psi = 0 \text{ on } \Omega\]
\[(\partial_n - B(k))\psi = 0 \text{ on } \partial \Omega\]

Resonance solutions are stationary points with respect to \(\psi\) of

\[\Phi(\psi, k) = \int_\Omega \left[ (\nabla \psi)^T (\nabla \psi) + \psi (V - k^2)\psi \right] \, d\Omega - \int_{\partial \Omega} \psi B(k)\psi \, d\Gamma\]

Discretized equations (e.g. via finite or spectral elements) are

\[A(k)\psi = \left( K - k^2 M - C(k) \right) \psi = 0\]

\(K\) and \(M\) are real symmetric and \(C(k)\) is complex symmetric.
This is still a little ugly:
- Nonlinear eigenproblems aren’t as nice as linear ones
- The DtN map is spatially nonlocal
  - Though on a circle, diagonalizable in Fourier modes

Maybe I can go back to linear eigenvalue problems?
- Essential singularity in $B(k)$ – can’t work everywhere ...
- ... but maybe I can control the error
Linear eigenproblems

Can also compute resonances by

- Adding a complex absorbing potential
- Complex scaling methods

Both result in complex-symmetric ordinary eigenproblems:

\[(K_{\text{ext}} - k^2 M_{\text{ext}}) \psi_{\text{ext}} = \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix} - k^2 \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0\]

where \(\psi_2\) correspond to extra variables (outside \(\Omega\)).
Eliminate “extra” variables $\psi_2$ to get

$$\hat{A}(k)\psi_1 = \left( K_{11} - k^2 M_{11} - \hat{C}(k) \right) \psi_1 = 0$$

where

$$\hat{C}(k) = (K_{12} - k^2 M_{12})(K_{22} - k^2 M_{22})^{-1}(K_{21} - k^2 M_{21})$$
Aside on spectral Schur complement

Inverse of a Schur complement is a submatrix of an inverse:

\[(K_{\text{ext}} - z^2 M_{\text{ext}})^{-1} = \begin{bmatrix} \hat{A}(z)^{-1} & * \\ * & * \end{bmatrix}\]

So for reasonable norms,

\[\|\hat{A}(z)^{-1}\| \leq \|(K_{\text{ext}} - z^2 M_{\text{ext}})^{-1}\|\].

Or

\[\Lambda_\epsilon(\hat{A}) \subset \Lambda_\epsilon(K_{\text{ext}}, M_{\text{ext}}),\]

\[\Lambda_\epsilon(\hat{A}) \equiv \{z : \|\hat{A}(z)^{-1}\| > \epsilon^{-1}\}\]
\[\Lambda_\epsilon(K_{\text{ext}}, M_{\text{ext}}) \equiv \{z : \|(K_{\text{ext}} - z^2 M_{\text{ext}})^{-1}\| > \epsilon^{-1}\}\]
Apples to oranges?

\[ A(k)\psi = (K - k^2M - C(k))\psi = 0 \quad \text{(exact DtN map)} \]
\[ \hat{A}(k)\psi = (K - k^2M - \hat{C}(k))\psi = 0 \quad \text{(spectral Schur complement)} \]

Two ideas:
- Perturbation theory for NEP for local refinement
- Complex analysis to get more global analysis

Will focus on the latter today.
To get axisymmetric resonances in corral model, compute:

- Eigenvalues of a complex-scaled problem
- Residuals in nonlinear eigenproblem
- \( \log_{10} \| A(k) - \hat{A}(k) \| \)

How do we know if we might miss something?
A little complex analysis

If $A$ nonsingular on $\Gamma$, analytic inside, count eigs inside by

$$W_\Gamma(\det(A)) = \frac{1}{2\pi i} \int_\Gamma \frac{d}{dz} \ln \det(A(z)) \, dz$$

$$= \text{tr} \left( \frac{1}{2\pi i} \int_\Gamma A(z)^{-1} A'(z) \, dz \right)$$

$E = A - \hat{A}$ also analytic inside $\Gamma$. By continuity,

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

if $A + sE$ nonsingular on $\Gamma$ for $s \in [0, 1]$. 
A general recipe

Analyticity of $A$ and $E$
Matrix nonsingularity test for $A + sE = $
Inclusion region for $\Lambda(A + E)$
Eigenvalue counts for connected components of region
Application: Matrix Rouché

\[ \| A(z)^{-1} E(z) \| < 1 \text{ on } \Gamma \iff \text{same eigenvalue count in } \Gamma \]

Proof:
\[ \| A(z)^{-1} E(z) \| < 1 \iff A(z) + sE(z) \text{ invertible for } 0 \leq s \leq 1. \]

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

Theorem
Let $S_\epsilon = \{ z : \| A(z) - \hat{A}(z) \| < \epsilon \}$. Any connected component of $\Lambda_\epsilon(K_{ext}, M_{ext})$ strictly inside $S_\epsilon$ contains the same number of eigenvalues for $A(k)$ and $\hat{A}(k)$.

Could almost certainly do better...
For more

More information at

http://www.cs.cornell.edu/~bindel/

- Links to tutorial notes on resonances with Maciej Zworski
- Matscat code for computing resonances for 1D problems
- These slides!