Resonances: Interpretation, Computation, and Perturbation

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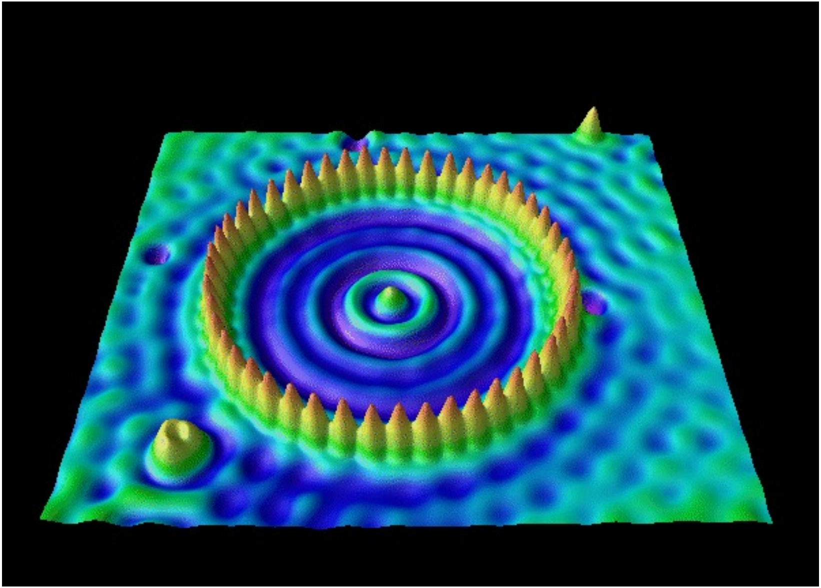
The quantum corral



Particle in a box

Time-harmonic Schrödinger equation:

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

where

$$V(x) = \begin{cases} 0, & 0 < x < 1 \\ \infty, & \text{otherwise.} \end{cases}$$

L^2 solutions exist for $E_n = k_n^2 = n^2\pi^2$:

$$\psi = \begin{cases} \sin(k_n x), & 0 < x < 1 \\ 0, & \text{otherwise.} \end{cases}$$

Particle in a box 2

Time-harmonic Schrödinger equation:

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

where

$$V(x) = \begin{cases} 0, & 0 < x < 1 \\ E_\infty, & \text{otherwise.} \end{cases}$$

L^2 solutions exist for discrete values below E_∞. Have the form

$$\psi = \begin{cases} A\exp(x\sqrt{E_\infty - E}), & x \leq 0 \\ B\sin(\sqrt{E}x) + C\cos(\sqrt{E}x), & 0 < x < 1 \\ D\exp((1-x)\sqrt{E_\infty - E}), & x \geq 0, \end{cases}$$

where ψ and ψ' are continuous (four constraints).

Particle in a box 3

Time-harmonic Schrödinger equation:

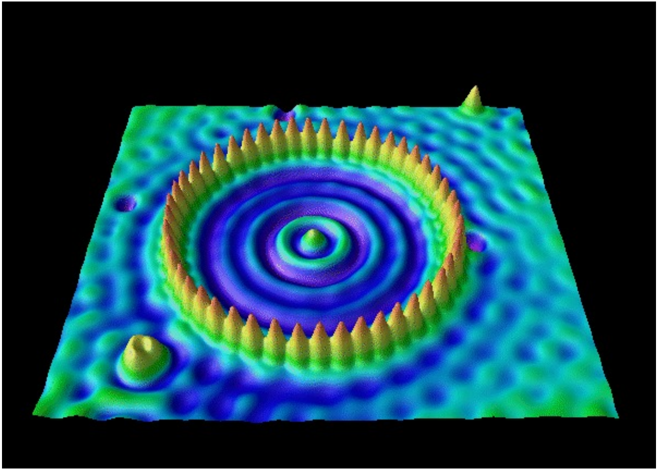
$$H\psi = \left(-\frac{d^2}{dx^2} + V\right)\psi = E\psi$$

where

$$V(x) = \begin{cases} 0, & 0 < x < 1 \\ E_\infty, & 1 < x < 1 + L \text{ and } -L < x < 0 \\ 0 & \text{otherwise.} \end{cases}$$

No L^2 solutions! But a two-parameter family of bounded "scattering solutions" for any $E = k^2 > 0$.

Electrons unbound



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

Scattering solutions

Schrödinger scattering from a potential V on $[a, b]$

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

For $E = k^2 > 0$, get solutions

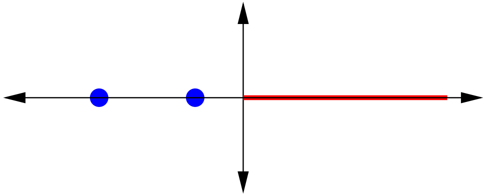
$$\psi = e^{-ikx} + \psi_{\text{scatter}}$$

where ψ_{scatter} satisfies outgoing BCs:

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

or via a *Dirichlet-to-Neumann* (DtN) map: $(\partial_n - B(k))\psi = 0$

Spectra and scattering

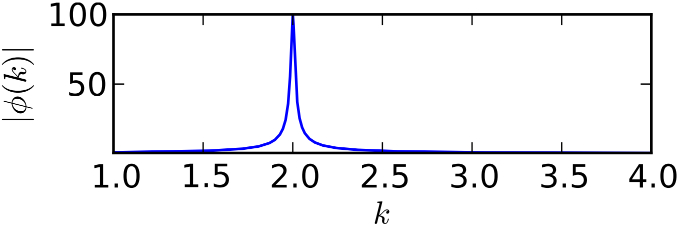


For compactly supported V, spectrum consists of

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

We're interested in the latter.

Resonances and scattering



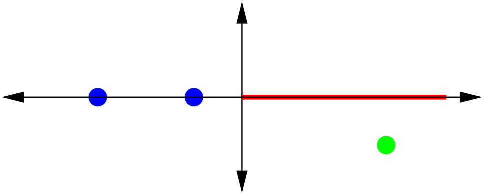
For $\text{supp}(V) \subset \Omega$, consider a scattering experiment:

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

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



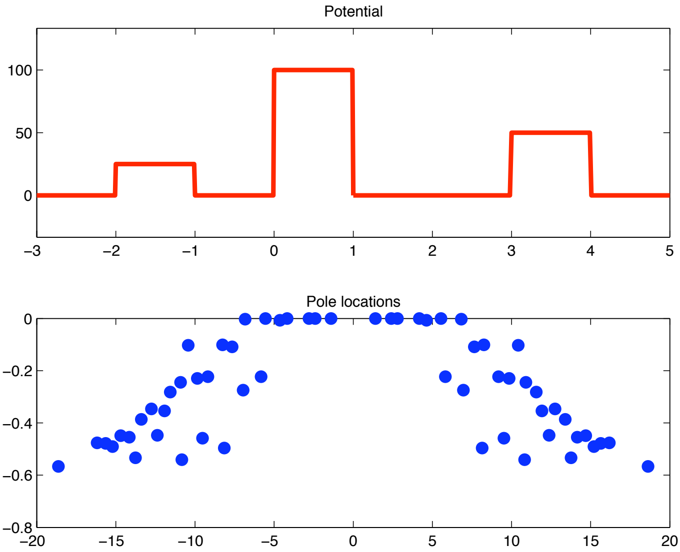
Consider a scattering measurement $\phi(k)$

- 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 ϕ
- Resonance poles are on a *second sheet of definition* for ϕ
- 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



Resonances and transients

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Eigenvalues and resonances

Eigenvalues	Resonances
Poles of resolvent	Second-sheet poles of extended resolvent
Vector in L^2	Wave function goes exponential
Stable states	Transients
Purely real	Imaginary part describes local decay

Computing resonances 1: Prony

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)

But this is numerically sensitive, may require long simulations.

Computing resonances 2: complex scaling

Change coordinates to shift the branch cut:

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

where $d\hat{x}/dx = 1 + i\sigma(x)$ is deformed outside $[a, b]$.

- Rotates the continuous spectrum to reveal resonances
- First used to *define* resonances (Simon 1979)
- Also a computational method:
  - Truncate to a finite $\tilde{x}$ domain.
  - Discretize using standard methods
  - Solve a complex symmetric eigenvalue problem

One of my favorite computational tactics.

Computing resonances 3: 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 ψ 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.

Computational tradeoffs

- Prony
  - Relatively simple signal processing
  - Can be used with scattering experiment results
  - May require long simulations
  - Numerically sensitive
- Complex scaling
  - Straightforward implementation
  - Yields a *linear* eigenvalue problem
  - How to choose scaling parameters, truncation?
- DtN map formulation
  - Bounded domain — no artificial truncation
  - Yields a *nonlinear* eigenvalue problem
  - DtN map is spatially nonlocal except in 1D (though diagonalized by Fourier modes on a circle)

The 1D case: MatScat

`http://www.cs.cornell.edu/~bindel/cims/matscat/`

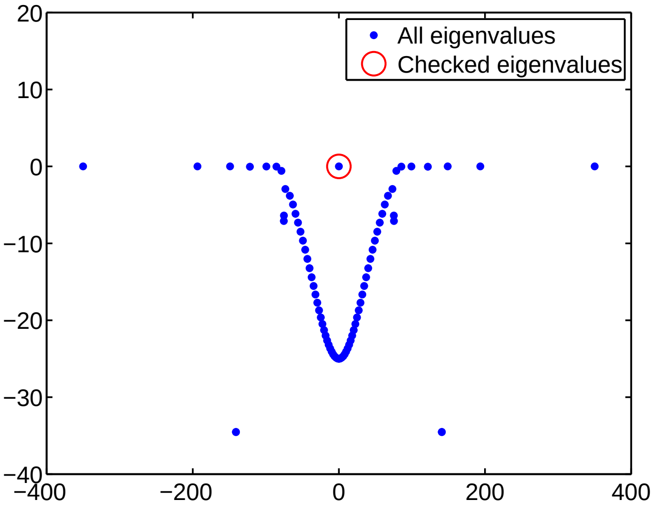
Basic MatScat strategy

Pseudospectral collocation at Chebyshev points:

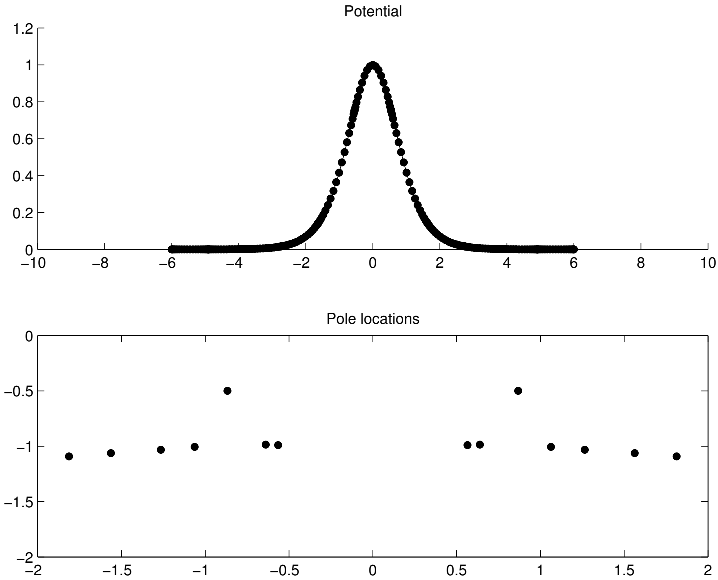
$$
\begin{aligned}
\left(-D^2 + V(x) - k^2\right)\psi &= 0, \quad x \in (a, b) \\
(D - ik)\,\psi &= 0, \quad x = b \\
(D + ik)\,\psi &= 0, \quad x = a
\end{aligned}
$$

Convert to linear problem with auxiliary variable $\phi = k\psi$.

Is it that easy?



Is it that easy?



Computation isn't enough!

Desired features:

- A method to compute all resonances in some region
- *and* some sense of the accuracy of the computation
- *and* some notion of sensitivity of the problem

Steps toward sensitivity

Resonance solutions are stationary points with respect to ψ of

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

If (ψ, k) a resonance pair, then $\Phi(\psi, k) = 0$ and $D_\psi \Phi(\psi, k) = 0$.

Potential perturbations

If (ψ, k) a resonance pair, then $\Phi(\psi, k) = 0$ and $D_\psi \Phi(\psi, k) = 0$.
What if we perturb V?

$$\delta\Phi = D_\psi \Phi \cdot \delta\psi + D_V \Phi \cdot \delta V + D_k \Phi \cdot \delta k = 0$$

Note that $D_\psi \Phi \cdot \delta\psi = 0$! So

$$\delta k = -\frac{D_V \Phi \cdot \delta V}{D_k \Phi}$$

Perturbation worked out

So look at how perturbations δV change k:

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

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

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

Backward error analysis in MatScat

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

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

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

But...

- Solving the 1D problem was only easy because it turned into a *quadratic* eigenvalue problem.
- In higher dimensions, get a more general nonlinear eigenvalue problem.
- Can I combine a linear eigenvalue problem with error analysis worked out using the DtN map?

Linear eigenproblems

Can also compute resonances by

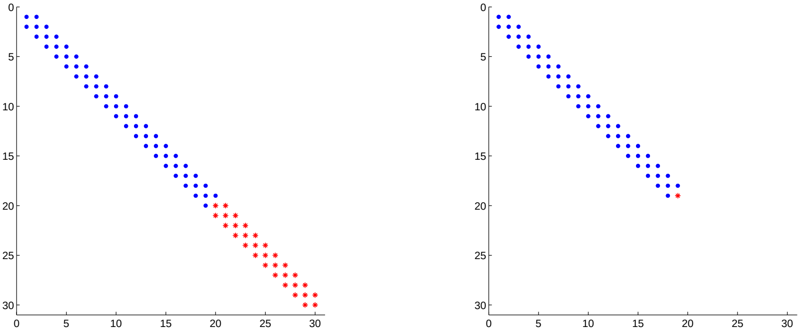
- Adding a complex absorbing potential
- Complex scaling methods

Both result in complex-symmetric ordinary eigenproblems:

$$(K_{ext} - k^2 M_{ext})\psi_{ext} = \left(\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} - k^2 \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \right) \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = 0$$

where ψ_2 correspond to extra variables (outside Ω).

Spectral Schur complement



Eliminate “extra” variables ψ_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:

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

So for reasonable norms,

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

Or

$$\Lambda_\epsilon(\hat{A}) \subset \Lambda_\epsilon(K_{ext}, M_{ext}),$$

$$\Lambda_\epsilon(\hat{A}) \equiv \{z : \|\hat{A}(z)^{-1}\| > \epsilon^{-1}\}$$
$$\Lambda_\epsilon(K_{ext}, M_{ext}) \equiv \{z : \|(K_{ext} - z^2 M_{ext})^{-1}\| > \epsilon^{-1}\}$$

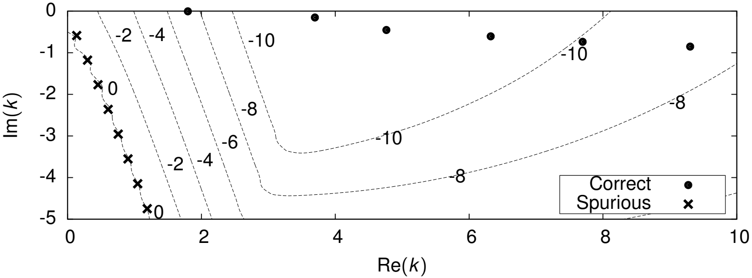
Apples to oranges?

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

Two ideas:

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

Linear vs nonlinear



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 Γ, analytic inside, count eigs inside by

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

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

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

if $A + sE$ nonsingular on Γ 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

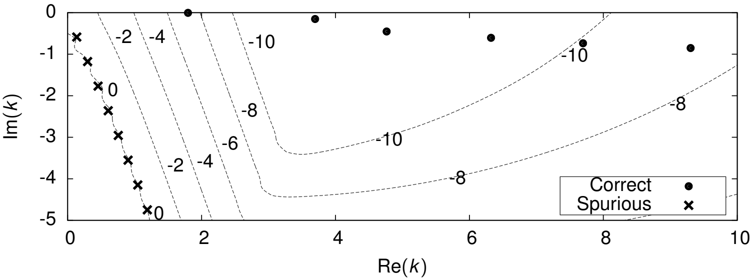
Application: Matrix Rouché

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

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

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

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_ϵ *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!