Resonances: Interpretation, Computation, and Perturbation

David Bindel and Maciej Zworski

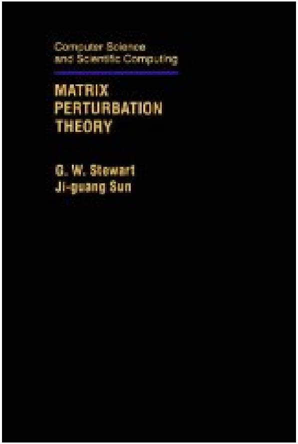
Department of Computer Science
Cornell University

Department of Mathematics
UC Berkeley

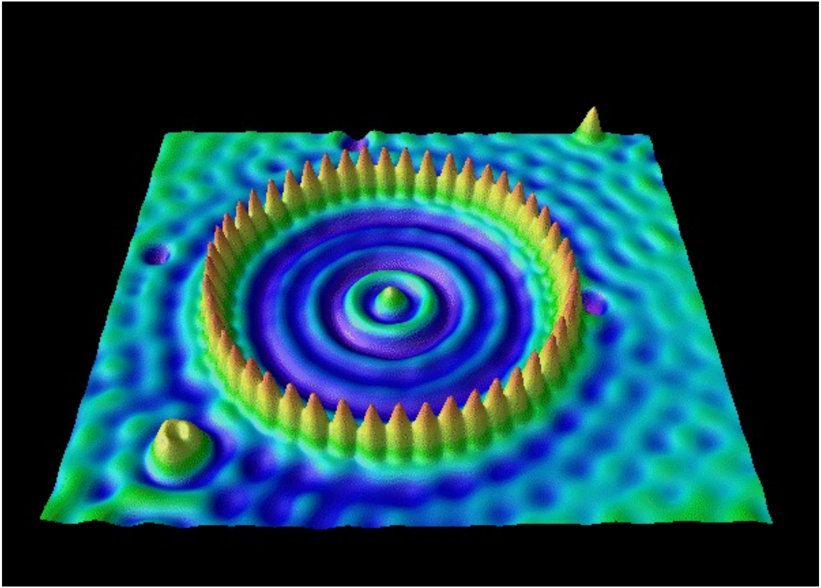
20 Jul 2010

Thanks, Pete!


AFTERNOTES ON NUMERICAL ANALYSIS
G. W. Stewart
AFTERNOTES goes to GRADUATE SCHOOL
Lectures on Advanced Numerical Analysis
siam
Matrix Algorithms
Stewart
Matrix Algorithms
Volume II: Eigensystems
G. W. Stewart
siam


Computer Science and Scientific Computing
MATRIX PERTURBATION THEORY
G. W. Stewart
Ji-guang Sun

The quantum corral



“Particle in a box” model

Schrödinger equation

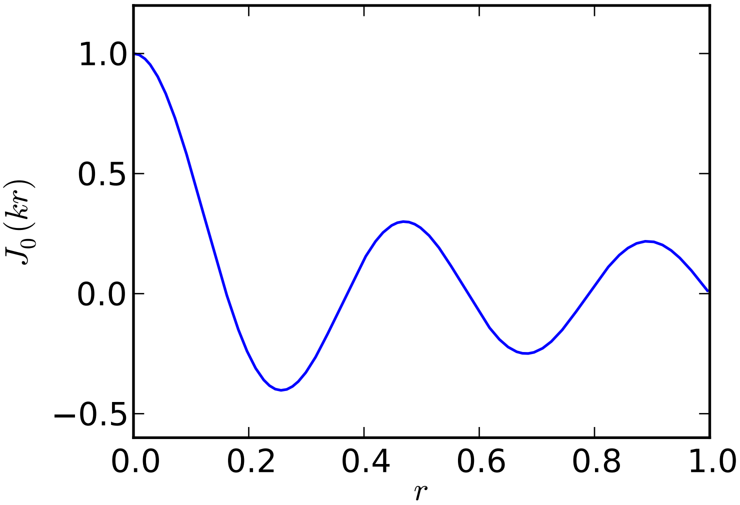
$$H\psi = (-\nabla^2 + V)\psi = E\psi$$

where

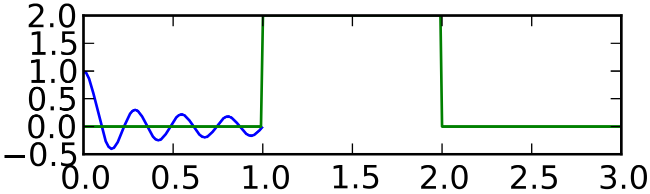
$$V(r) = \begin{cases} 0, & r < 1 \\ \infty, & r \geq 1 \end{cases}$$

Result: eigenmodes of Laplace with Dirichlet BC.

Eigenfunctions at the quantum corral



A more realistic model?

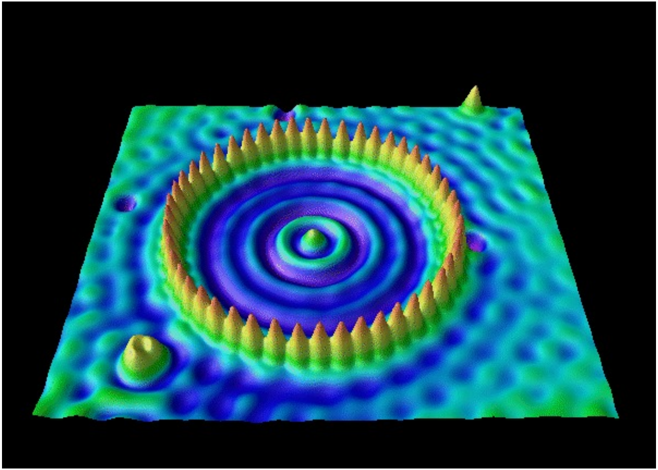


Corral really looks like a *finite* potential

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

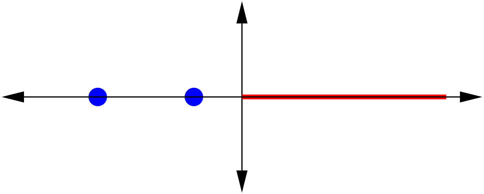
Does anything change?

Electrons unbound



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

Spectra and scattering

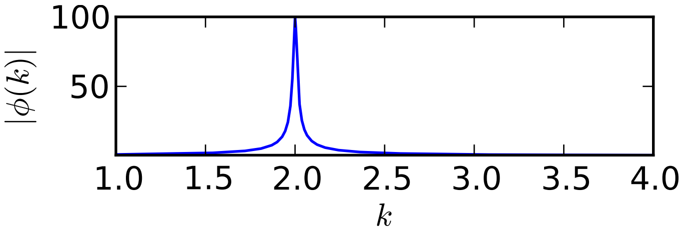


For compactly supported V, spectrum consists of

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

We're interested in the latter.

Resonances and scattering



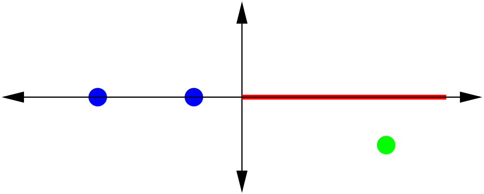
For supp$(V) \subset \Omega$, consider a scattering experiment:

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

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



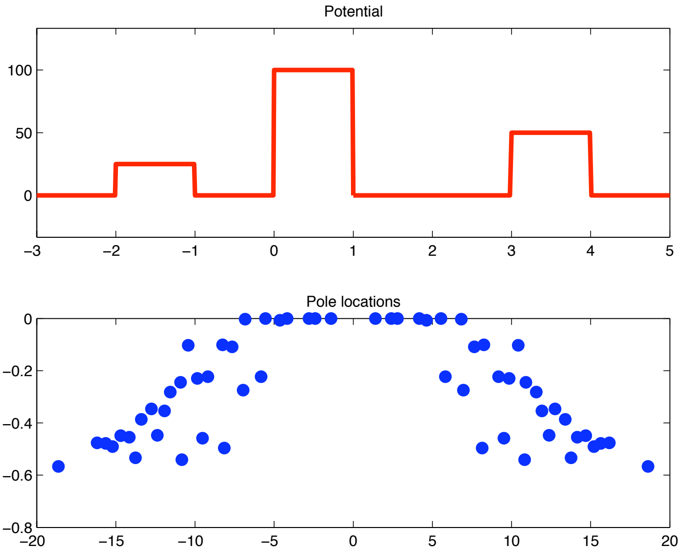
Consider a scattering measurement $\phi(k)$

- 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

(Loading outs.mp4)

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

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 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.

Humbug!

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

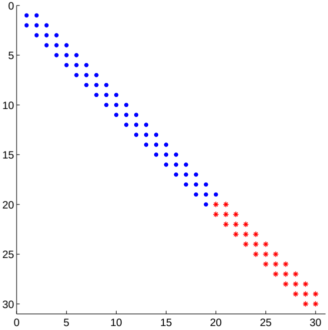
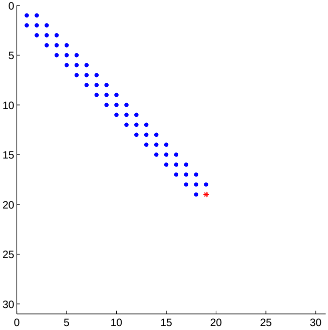
- Adding a complex absorbing potential
- Complex scaling methods

Both result in complex-symmetric ordinary eigenproblems:

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

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?

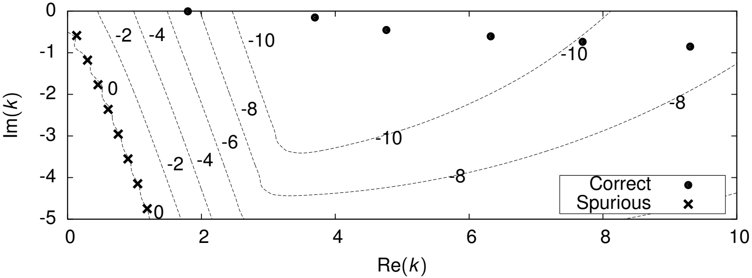
$$A(k)\psi = (K - k^2 M - C(k))\psi = 0 \quad \text{(exact DtN map)}$$
$$\hat{A}(k)\psi = (K - k^2 M - \hat{C}(k))\psi = 0 \quad \text{(spectral Schur complement)}$$

Two ideas:

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

Will focus on the latter today.

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

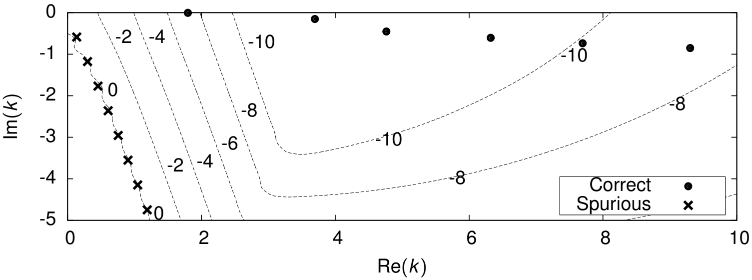
Application: Matrix Rouché

$\|A(z)^{-1}E(z)\| < 1$ 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!