Analyzing Resonances via Nonlinear Eigenvalues

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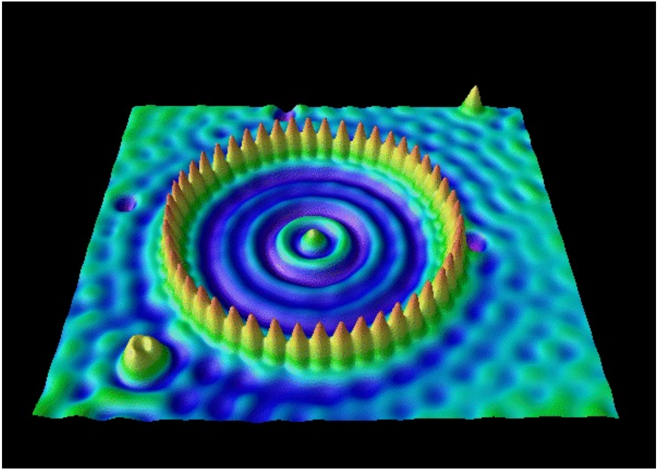
The quantum corral



(Crommie, Lutz, Eigler 1993 – iron on copper)

“Particle in a box” model

Schrödinger equation

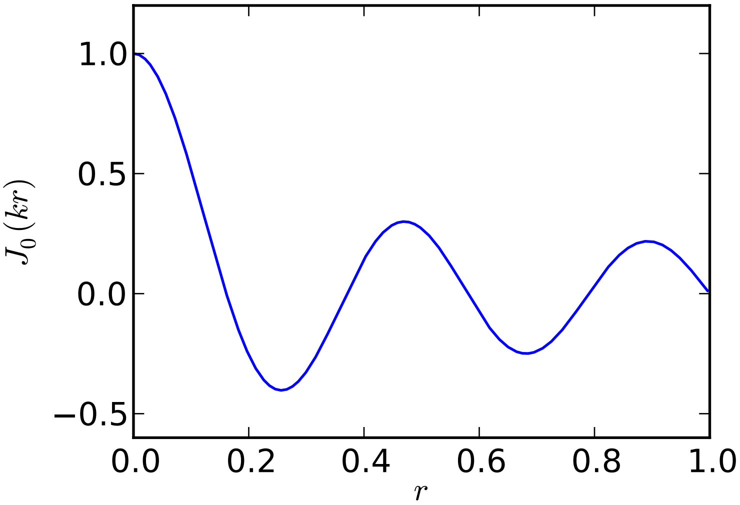
$$H\psi = (-\nabla^2 + V)\psi = E\psi$$

where

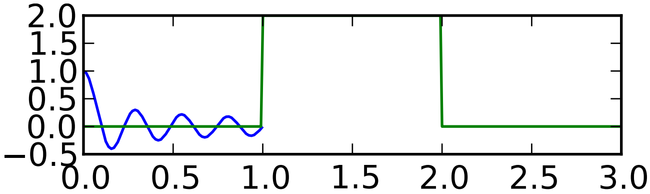
$$V(r) = \begin{cases} 0, & r < 1 \\ \infty, & r \geq 1 \end{cases}$$

Result: eigenmodes of Laplace with Dirichlet BC.

Eigenfunctions at the quantum corral



A more realistic model?

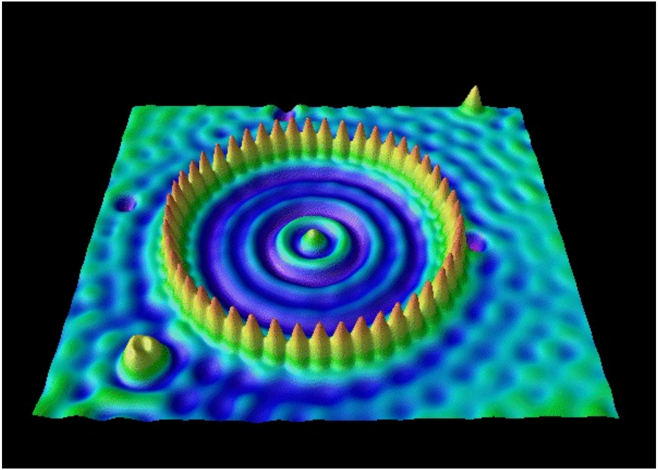


Corral really looks like a *finite* potential

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

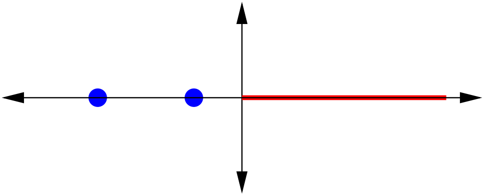
Does anything change?

Electrons unbound



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

Spectra and scattering

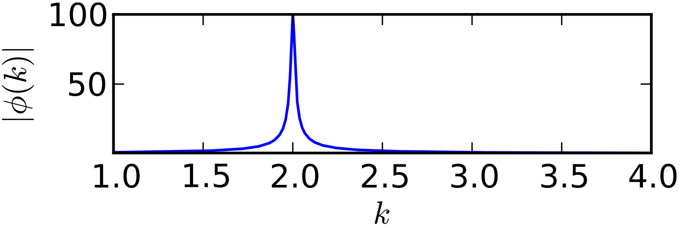


For compactly supported V, spectrum consists of

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

We're interested in the latter.

Resonances and scattering



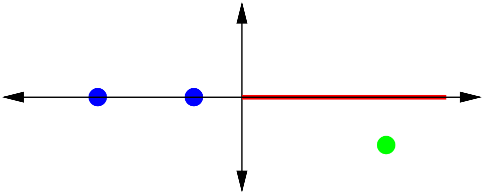
For $\text{supp}(V) \subset \Omega$, consider a scattering experiment:

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

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 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

From "Listening To A Monk From Shu Playing The Lute,"
interpreted by Vikram Seth, Three Chinese Poets*, 1993*

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:

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

where $B(k)$ is a (nonlocal) Dirichlet-to-Neumann map.

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.

One-dimensional resonances: a special case

The one-dimensional case is very nice:

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

- Get a quadratic eigenvalue problem in k
- Pseudospectral collocation scheme exactly satisfies BCs
- Have backward error analysis for discretization error based on a perturbed potential $\hat{V}$
- Have a robust MATLAB code (Matscat)

Things get harder in more than one dimension

Solution strategies

- Newton-like (local) methods
  - Can go beyond linear approximation (Kressner, Botchev)
  - Can miss things (near-multiple eigenvalues are common)
- Complex analytic methods
  - Contour integration (Beyn, Sakurai-Sugiura) or
    Taylor expansion (Jarlebring-Michiels-Meerbergen)
  - Choose a good contour and quadrature?
    Compute lots of Taylor terms?
- Approximate radiating boundary conditions
  - Linear (or rational) eigenproblems
  - How does it compare to NEP (spurious/missing soutions?)

Approximate BCs and linear eigenproblems

Can also compute resonances by

- Adding a complex absorbing potential
- Complex scaling methods

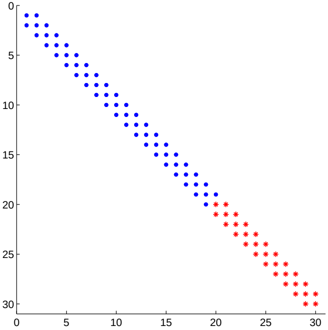
Both result in complex-symmetric ordinary eigenproblems:

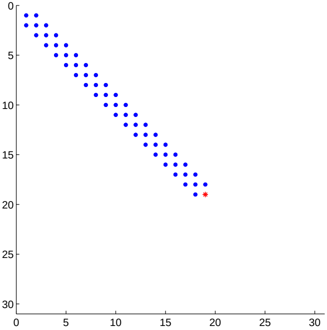
$$(K_{ext} - k^2 M_{ext})\psi_{ext} = \left(\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} - k^2 \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \right) \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = 0$$

where ψ_2 correspond to extra variables (outside Ω).

How do I compare this to the NEP?

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

$$\hat{C}(k) = (K_{12} - k^2 M_{12})(K_{22} - k^2 M_{22})^{-1}(K_{21} - k^2 M_{21})$$

Evaluating the boundary approximation

Think of LEP approximating NEP via Schur complement:

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

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

Want stability of NEP solutions + small $E(k) = C(k) - \hat{C}(k)$.
Then apply perturbation theory to the NEP (done in Matscat).

Evaluating the boundary approximation

Or think of NEP approximating LEP:

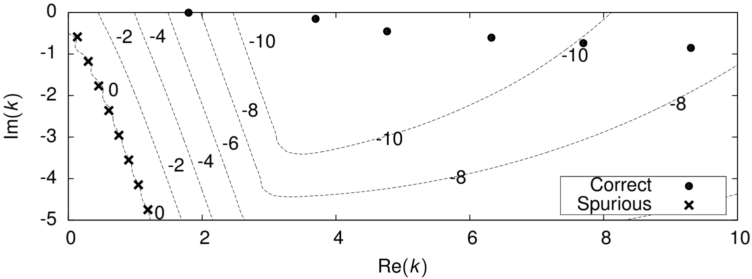
$$\hat{A}_{\text{ext}}(k)\hat{\psi}_{\text{ext}} = (K_{\text{ext}} - k^2 M_{\text{ext}} \qquad\qquad)\hat{\psi}_{\text{ext}} = 0$$

$$A_{\text{ext}}(k)\psi_{\text{ext}} = (K_{\text{ext}} - k^2 M_{\text{ext}} + E_{\text{ext}}(k))\psi_{\text{ext}} = 0$$

Point: Error analysis of the *nonlinear* eigenproblem from

- Bounds on $E_{\text{ext}}(k)$ (or on a residual)
- Stability information for the *linear* eigenproblem
- A smattering of complex analysis

Linear vs nonlinear



(Eigenvalues from complex scaling + contours of $\log_{10} \|E(k)\|$)

To find axisymmetric resonances in corral model:

- Compute eigenvalues of a complex-scaled problem
- Bound error $E(k)$ due to DtN map approximation
- Check sensitivity of linear eigenvalue problem

First-order analysis

Suppose $(K_{\text{ext}} - \hat{k}^2 M_{\text{ext}})\hat{\psi}_{\text{ext}} = 0$ and $E_{\text{ext}}(\hat{k})$ small.
If $k = \hat{k} + \delta k$ a resonance, then to first order

$$\delta k = \frac{1}{2\hat{k}} \left(\frac{\hat{\psi}_{\text{ext}}^T \, E_{\text{ext}}(\hat{k}) \, \hat{\psi}_{\text{ext}}}{\hat{\psi}_{\text{ext}}^T \, M_{\text{ext}} \, \hat{\psi}_{\text{ext}}} \right) = \frac{1}{2\hat{k}} \left(\frac{\hat{\psi}_{\text{ext}}^T \, (A_{\text{ext}}(\hat{k}) \, \hat{\psi}_{\text{ext}})}{\hat{\psi}_{\text{ext}}^T \, M_{\text{ext}} \, \hat{\psi}_{\text{ext}}} \right)$$

This lets us

- Refine good approximate resonances.
- Discard spurious eigenvalues.

But could we miss anything?

Global analysis

Consider

$$\hat{A}_s(k) = (K_{\text{ext}} - k^2 M_{\text{ext}} + sE_{\text{ext}}(k)).$$

Eigenvalues of $\hat{A}_s(k)$ are continuous (in domain of analyticity). Therefore:

- Resonances inside $D_\epsilon = \{z : \|E_{\text{ext}}(z)\| < \epsilon\}$ must lie in a structured ϵ-pseudospectrum for the linear eigenproblem.
- If $U \subset \text{interior}(D_\epsilon)$ a connected component of structured ϵ-pseudospectrum, then U contains the same number of linear eigenvalues and resonances.

Current directions

- Rational approximation to an NEP gives approximate solutions *and* a basis for backward error analysis
- Current work (with Amanda Hood):
  - Study of how other artificial BCs approximate DtN
  - Incorporate discretization error, linear eigensolver error, boundary condition approximation in same framework

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!

Thanks to:

- Maciej Zworski
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