Numerical Methods for Resonance Calculations

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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 $\operatorname{supp}(V) \subset [a, b]$, write

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

$\operatorname{Im} k \geq 0$ for eigenvalues, $\operatorname{Im} k < 0$ for resonances.

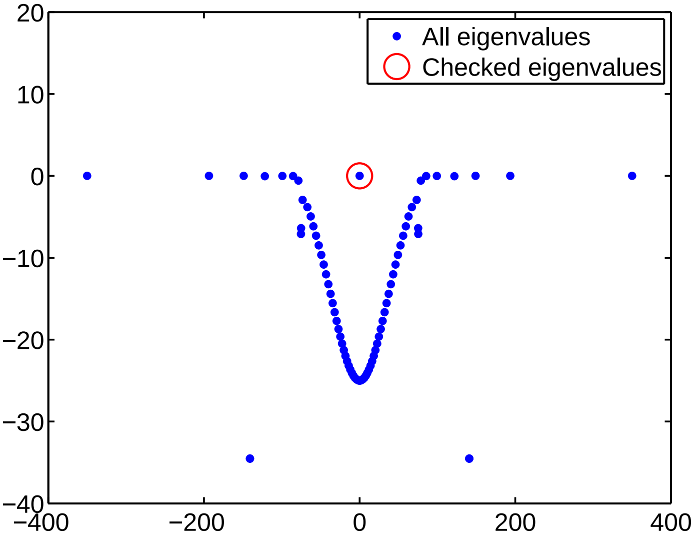
Pseudospectral Discretization

Sample ψ 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?



Backward Error Analysis

If $\hat{\psi}$ is a numerical solution, there is some $\hat{V}$ s.t.

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

First-order sensitivity to changes in $\hat{V}$ is

$$\delta k = \frac{\int_a^b \hat{\psi}(\delta V)\hat{\psi}}{2k\int_a^b \hat{\psi}^2 + i(\hat{\psi}^2(a) + \hat{\psi}^2(b))}$$
$$= \frac{\int_a^b \hat{\psi}(H_V - k^2)\hat{\psi}}{2k\int_a^b \hat{\psi}^2 + i(\hat{\psi}^2(a) + \hat{\psi}^2(b))}.$$

Compute $\hat{V}$ by evaluating residual for approximate $\hat{\psi}$ on a fine mesh.

Backward Error Analysis

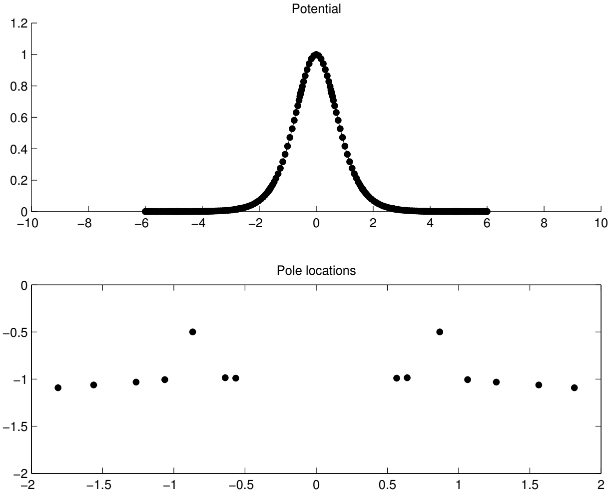
First-order sensitivity to changes in $\hat{V}$ is

$$\delta k = \frac{\int_a^b \hat{\psi}(\delta V)\hat{\psi}}{2k \int_a^b \hat{\psi}^2 + i(\hat{\psi}^2(a) + \hat{\psi}^2(b))}.$$

Now think about perturbing from a truncated potential to a non-compactly supported potential. Above bound says this is okay as long as $|V|/\exp(2\,\mathrm{Im}(k)|x|) \rightarrow 0$ as $|x| \rightarrow \infty$.

Backward Error Analysis

Example: truncate Eckart potential $\cosh^{-2}(x)$



Matscat

- `http://www.cims.nyu.edu/~dbindel/matscat`
- Toolbox for 1D Schrödinger scattering and resonances
- Piecewise smooth, compactly supported potentials
- Computes resonances and scattered fields
- The `demo.m` file runs all demonstrations