# Resonance sensitivity for Schrödinger

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## 1 A perturbation result

Start with the Schrödinger equation with a potential $V$ compactly supported inside $(a, b)$, and replace the equation outside the $(a, b)$ with appropriate boundary conditions:

$$\begin{aligned}(H-\lambda^2)\psi &= 0 \text{ for } x \in (a,b) &(1)\\ (\partial_x - i\lambda)\psi &= 0 \text{ at } x = b &(2)\\ (\partial_x + i\lambda)\psi &= 0 \text{ at } x = a. &(3)\end{aligned}$$

Values of $\lambda$ in the upper half plane correspond to eigenvalues of the original problem; values in the lower half plane correspond to resonances.

Now suppose $\delta V$ is a perturbing potential supported inside $(a, b)$. Taking variations, we have

$$\begin{aligned}(H-\lambda^2)\delta\psi + (\delta V - 2\lambda\delta\lambda)\psi &= 0 \text{ for } x \in (a,b) &(4)\\ (\partial_x - i\lambda)\delta\psi - i\delta\lambda\psi &= 0 \text{ at } x = b &(5)\\ (\partial_x + i\lambda)\delta\psi + i\delta\lambda\psi &= 0 \text{ at } x = a. &(6)\end{aligned}$$

Integrating by parts, we have

$$\begin{aligned}\int_a^b \psi(H-\lambda^2)\delta\psi &= \left[-\psi\partial_x\delta\psi + \partial_x\psi\delta\psi\right]_a^b + \int_a^b \delta\psi(H-\lambda^2)\psi &(7)\\ &= \left[-\psi\partial_x\delta\psi + \partial_x\psi\delta\psi\right]_a^b. &(8)\end{aligned}$$

Using the boundary conditions, we now have that

$$\begin{aligned}\left[-\psi\partial_x\delta\psi + \partial_x\psi\delta\psi\right]_a^b. &= \left[-\psi(\pm i\lambda\delta\psi \pm i\delta\lambda\psi) + (\pm i\lambda\psi\delta\psi)\right]_a^b &(9)\\ &= \left[\mp i\delta\lambda\psi^2\right]_a^b &(10)\\ &= -i\delta\lambda(\psi(a)^2 + \psi(b)^2). &(11)\end{aligned}$$

Therefore when we integrate the domain variational equation against $\psi$, we have

$$\begin{aligned}0 &= \int_a^b \left\{\psi(H-\lambda^2)\delta\psi + \psi(\delta V - 2\lambda\delta\lambda)\psi\right\} &(12)\\ &= -i\delta\lambda(\psi(a)^2 + \psi(b)^2) + \int_a^b \delta V\psi^2 - 2\lambda\delta\lambda\int_a^b \psi^2. &(13)\end{aligned}$$

so that

$$\delta\lambda = \frac{\int_a^b \delta V \psi^2}{2\lambda \int_a^b \psi^2 + i(\psi^2(a) + \psi^2(b))}. \tag{14}$$

## 2 Application to potential cutoff

Now consider the denominator in (14). If the support of $V$ is contained in $(a, b)$ and the support of our perturbation is contained in a larger interval $(A, B)$, then we know that

$$\psi(x) = \begin{cases} c_+ e^{i\lambda x} & \text{for } b < x \\ c_- e^{-i\lambda x} & \text{for } x < a \end{cases} \tag{15}$$

Therefore, we can write

$$\begin{aligned}
\int_A^B \psi^2 &= \int_A^a c_-^2 e^{-2i\lambda x} + \int_b^B c_+^2 e^{2i\lambda x} + \int_a^b \psi^2 && (16)\\
&= \frac{1}{2i\lambda}\left(c_+^2 e^{2i\lambda B} + c_-^2 e^{-2i\lambda A}\right) && (17)\\
&\quad -\frac{1}{2i\lambda}\left(c_+^2 e^{2i\lambda b} + c_-^2 e^{-2i\lambda a}\right) + \int_a^b \psi^2 && (18)\\
&= \frac{-i}{2\lambda}\left(\psi(B)^2 + \psi(A)^2\right) + \frac{i}{2\lambda}\left(\psi(b)^2 + \psi(a)^2\right) + \int_a^b \psi^2. && (19)
\end{aligned}$$

Therefore we have

$$\begin{aligned}
&\left(2\lambda \int_A^B \psi^2\right) + i(\psi(B)^2 + \psi(A)^2) \\
&= \left(2\lambda \int_a^b \psi^2 - i(\psi(B)^2 + \psi(A)^2) + i(\psi(a)^2 + \psi(b)^2)\right) \\
&\quad + i(\psi(B)^2 + \psi(A)^2) \\
&= 2\lambda \int_a^a \psi^2 + i(\psi(b)^2 + \psi(a)^2)
\end{aligned}$$

Thus the denominator in the perturbation bound is *independent* of the interval $(A, B)$ supporting $\delta V$; it depends only on the interval $(a, b)$. So for a support on a larger interval $(A, B)$, we have

$$\delta\lambda = \frac{\int_A^B \delta V \psi^2}{2\lambda \int_a^b \psi^2 + i(\psi^2(a) + \psi^2(b))}. \tag{20}$$

Now suppose we take the limiting case where the perturbation $\delta V$ is supported on the entire real line. For example, we might be interested in what happens when we compute resonances by applying a cutoff to the potential, so that the perturbation corresponds to everything that we have cut off. Then the

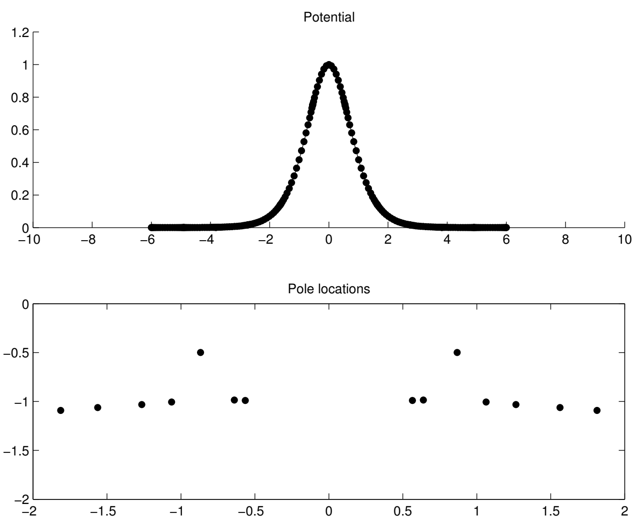


Figure 1: Computed resonances for an Eckart potential. Because the potential is truncated to a finite interval, only resonances above the line $\Im(\lambda) = -1$ need correspond to true resonances for the original potential supported on all of $\mathbb{R}$.

above bound says, roughly, that we can only treat the truncated potential as "close to" the true potential when the true potential decays sufficiently faster than $e^{2\Im(\lambda)|x|}$ as $|x| \to \infty$.

As a concrete case, let us consider an Eckart barrier

$$V_E(x) = \cosh(x)^{-2}. \tag{21}$$

In order to compute resonances for the potential $V_E$, we write $V_E = V + \delta V$, where $V = V_E$ on some bounded interval $(a, b)$ and $V = 0$ outside that interval. We would now like to claim that $\delta V$ is a small perturbation, so that computing resonances from the truncated potential $V$ gives us an approximation to resonances of the original potential $V_E$. But the integral expression for $\delta\lambda$ above (with $A = -\infty$ and $B = \infty$) can only converge when $\Im(\lambda) > -1$. Indeed, when computing resonances for the Eckart potential by truncating to a compactly supported potential, we are only able to resolve the resonances above the line $\Im(\lambda) = -1$; around $\Im(\lambda) = -1$, the truncated potential has many spurious resonances which effectively mask the behavior of any resonances for $V_E$ which might live deeper in the complex plane (Figure 1).

## 3 Numerical sensitivity analysis

Now suppose that we have computed an approximate resonant state $(\hat{\psi}, \lambda)$ by a pseudospectral collocation discretization of (1)-(3). Then $\hat{\psi}$ exactly satisfies

$$\begin{aligned}
(\hat{H} - \lambda^2)\psi &= 0 \text{ for } x \in (a,b) && (22)\\
(\partial_x - i\lambda)\psi &= 0 \text{ at } x = b && (23)\\
(\partial_x + i\lambda)\psi &= 0 \text{ at } x = a. && (24)
\end{aligned}$$

where $\hat{H} = H + \delta V = H - \hat{\psi}^{-1} R$ with $R := (H - \lambda^2)\psi$ the residual. Assuming $\delta V$ is small and $\lambda$ is reasonably isolated, the error in the computed $\lambda$ will be approximately

$$\delta\lambda = \frac{\int_a^b \hat{\psi} R}{2\lambda \int_a^b \hat{\psi}^2 + i(\hat{\psi}^2(a) + \hat{\psi}^2(b))}. \tag{25}$$

We can approximate this formula directly by numerical integration; we need only to be sure that $R$ is sampled with adequate density, since by definition $R$ is zero at the points associated with the original collocation grid.

## 4 Perturbation in higher dimensions

Now consider the more general case of a Schrödinger equation in $\mathbb{R}^n$ with a potential inside some finite domain $\Omega$ with appropriate Dirichlet-to-Neumann boundary conditions

$$\begin{aligned}
(H - \lambda^2)\psi &= 0 \text{ for } x \in \Omega && (26)\\
\frac{\partial \psi}{\partial n} - B(\lambda)\psi &= 0 \text{ for } x \in \Gamma = \partial\Omega. && (27)
\end{aligned}$$

As before, suppose $\delta V$ is a perturbing potential supported inside $\Omega$; then taking variations, we have

$$\begin{aligned}
(H - \lambda^2)\delta\psi + (\delta V - 2\lambda\delta\lambda) &= 0 \text{ for } x \in \Omega && (28)\\
\frac{\partial \delta\psi}{\partial n} - B(\lambda)\delta\psi + B'(\lambda)\psi\delta\lambda &= 0 \text{ for } x \in \Gamma = \partial\Omega. && (29)
\end{aligned}$$

As before, we will multiply the domain equation by $\psi$ and integrate by parts. The key term is

$$\begin{aligned}
\int_\Omega \psi(H - \lambda^2)\delta\psi &= -\int_\Gamma \left(\psi \frac{\partial \delta\psi}{\partial n} - \delta\psi \frac{\partial \psi}{\partial n}\right) + \int_\Omega \delta\psi (H - \lambda^2)\psi && (30)\\
&= -\int_\Gamma (\psi B(\lambda)\delta\psi + \psi B'(\lambda)\psi\delta\lambda - \delta\psi B(\lambda)\psi) && (31)\\
&= -\int_\Gamma \psi B'(\lambda)\psi\delta\lambda. && (32)
\end{aligned}$$

Therefore when we integrate the domain variational equation against $\psi$, we have

$$\begin{aligned} 0 &= \int_\Omega \psi(H-\lambda^2)\delta\psi + \psi(\delta V - 2\lambda\delta\lambda)\psi && (33)\\ &= -\int_\Gamma \psi B'(\lambda)\psi\delta\lambda + \int_\Omega \psi(\delta V - 2\lambda\delta\lambda)\psi, && (34)\end{aligned}$$

which we can rearrange to obtain

$$\delta\lambda = \frac{\int_\Omega \delta V \psi^2}{2\lambda\int_\Omega \psi^2 + \int_\Gamma \psi B'(\lambda)\psi}. \tag{35}$$

If we were to also allow a perturbation in the DtN map (e.g. in order to analyze the effects of approximate absorbing boundary conditions), we would have

$$\delta\lambda = \frac{\int_\Omega \delta V \psi^2 + \int_\Gamma \psi \delta B \psi}{2\lambda\int_\Omega \psi^2 + \int_\Gamma \psi B'(\lambda)\psi}. \tag{36}$$

# 5 Domain independence of the denominator

Now suppose that $\phi(x,\lambda)$ is the solution to a Dirichlet problem

$$\begin{aligned} \left(\Delta+\lambda^2\right)\phi &= 0 \text{ on } \Omega && (37)\\ \phi &= f \text{ on } \Gamma = \partial\Omega && (38)\\ \frac{\partial\phi}{\partial n} &= B(\lambda)f \text{ on } \Gamma && (39)\end{aligned}$$

where $B(\lambda)$ is an appropriate Dirichlet-to-Neumann map. Taking variations with respect to $\lambda$ gives us the problem

$$\begin{aligned} (\Delta+\lambda^2)\delta\phi + 2\lambda\delta\lambda\phi &= 0 \text{ on } \Omega && (40)\\ \delta\phi &= 0 \text{ on } \Gamma && (41)\\ \frac{\partial\delta\phi}{\partial n} &= B(\lambda)\delta\phi + B'(\lambda)f\delta\lambda && (42)\\ &= B'(\lambda)f\delta\lambda && (43)\\ &= B'(\lambda)\phi\delta\lambda \text{ on } \Gamma. && (44)\end{aligned}$$

Integrating the domain equation against $\phi$ now gives

$$\int_\Omega \phi(\Delta+\lambda^2)\delta\phi + 2\lambda\delta\lambda\int_\Omega \phi^2 = 0. \tag{45}$$

If we integrate the first term by parts twice, we have

$$\begin{aligned}
&\int_\Omega \phi(\Delta+\lambda^2)\delta\phi \\
&\quad = \int_\Gamma \left(\phi\frac{\partial\delta\phi}{\partial n} - \delta\phi\frac{\partial\phi}{\partial n}\right) + \int_\Omega \delta\phi(\Delta+\lambda^2)\phi \\
&\quad = \int_\Gamma \phi\frac{\partial\delta\phi}{\partial n} \\
&\quad = \delta\lambda\int_\Gamma \phi B'(\lambda)\phi.
\end{aligned}$$

Therefore

$$2\lambda\int_\Omega \phi^2 + \int_\Gamma \phi B'(\lambda)\phi = 0. \tag{46}$$

Because the wave function $\psi$ from the previous section will satisfy a Helmholtz equation outside the support of $V$, equation (46) implies that the denominator of (36) is independent of the integration domain $\Omega$, beyond the fact that said integration domain should contain the support of $V$.