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{align*}
(H - \lambda^2)\psi &= 0 \text{ for } x \in (a, b) \\
(\partial_x - i\lambda)\psi &= 0 \text{ at } x = b \\
(\partial_x + i\lambda)\psi &= 0 \text{ at } x = a.
\end{align*}

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{align*}
(H - \lambda^2)\delta\psi + (\delta V - 2\lambda\delta\lambda)\psi &= 0 \text{ for } x \in (a, b) \\
(\partial_x - i\lambda)\delta\psi - i\delta\lambda\psi &= 0 \text{ at } x = b \\
(\partial_x + i\lambda)\delta\psi + i\delta\lambda\psi &= 0 \text{ at } x = a.
\end{align*}

Integrating by parts, we have

\begin{align*}
\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 \\
&= \left[ -\psi \partial_x \delta\psi + \partial_x \psi \delta\psi \right]_a^b.
\end{align*}

Using the boundary conditions, we now have that

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

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

\begin{align*}
0 &= \int_a^b \{ \psi (H - \lambda^2)\delta\psi + \psi (\delta V - 2\lambda\delta\lambda)\psi \} \\
&= -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.
\end{align*}
so that

\[ \delta \lambda = \frac{\int_a^b \delta V \psi^2}{2 \lambda \int_a^b \psi^2 + i(\psi^2(a) + \psi^2(b))}. \]  

(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

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

(15)

Therefore, we can write

\[ \int_A^B \psi^2 = \int_A^a c_+^2 e^{-2i \lambda x} + \int_b^B c_+^2 e^{2i \lambda x} + \int_b^a \psi^2 \]  

(16)

\[ = \frac{1}{2i \lambda} \left( c_+^2 e^{2i \lambda B} + c_-^2 e^{-2i \lambda A} \right) \]  

(17)

\[ - \frac{1}{2i \lambda} \left( c_+^2 e^{2i \lambda b} + c_-^2 e^{-2i \lambda a} \right) + \int_a^b \psi^2 \]  

(18)

\[ = \frac{-i}{2 \lambda} (\psi(B)^2 + \psi(A)^2) + \frac{i}{2 \lambda} (\psi(b)^2 + \psi(a)^2) + \int_a^b \psi^2. \]  

(19)

Therefore we have

\[ \left(2 \lambda \int_A^B \psi^2 \right) + i(\psi(B)^2 + \psi(A)^2) \]  

\[ = \left(2 \lambda \int_a^b \psi^2 - i(\psi(B)^2 + \psi(A)^2) + i(\psi(a)^2 + \psi(b)^2) \right) \]  

\[ + i(\psi(B)^2 + \psi(A)^2) \]  

\[ = 2 \lambda \int_a^b \psi^2 + i(\psi(b)^2 + \psi(a)^2) \]

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

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

(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

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

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
\[
(\hat{H} - \lambda^2)\psi = 0 \text{ for } x \in (a, b)
\]
\[
(\partial_x - i\lambda)\psi = 0 \text{ at } x = b
\]
\[
(\partial_x + i\lambda)\psi = 0 \text{ at } x = a.
\]

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

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

\[
(H - \lambda^2)\psi = 0 \text{ for } x \in \Omega
\]
\[
\frac{\partial\psi}{\partial n} - B(\lambda)\psi = 0 \text{ for } x \in \Gamma = \partial\Omega.
\]

As before, suppose \(\delta V\) is a perturbing potential supported inside \(\Omega\); then taking variations, we have
\[
(H - \lambda^2)\delta \psi + (\delta V - 2\lambda\delta \lambda) = 0 \text{ for } x \in \Omega
\]
\[
\frac{\partial\delta \psi}{\partial n} - B(\lambda)\delta \psi + B'(\lambda)\psi \delta \lambda = 0 \text{ for } x \in \Gamma = \partial\Omega.
\]

As before, we will multiply the domain equation by \(\psi\) and integrate by parts. The key term is
\[
\int_{\Omega} \psi(H - \lambda^2)\delta \psi = -\int_{\Gamma} \left( \psi \frac{\partial \delta \psi}{\partial n} - \delta \psi \frac{\partial \psi}{\partial n} \right) + \int_{\Omega} \delta \psi(H - \lambda^2)\psi
\]
\[
= -\int_{\Gamma} (\psi B(\lambda)\delta \psi + \psi B'(\lambda)\psi \delta \lambda - \delta \psi B(\lambda)\psi) + \int_{\Omega} \delta \psi B'(\lambda)\psi \delta \lambda.
\]
Therefore when we integrate the domain variational equation against $\psi$, we have
\begin{align}
0 &= \int_{\Omega} \psi(H - \lambda^2) \delta \psi + \psi(\delta V - 2\lambda \delta \lambda) \psi \\
&= -\int_{\Gamma} \psi B'(\lambda) \delta \lambda + \int_{\Omega} \psi (\delta V - 2\lambda \delta \lambda) \psi, \quad (33)
\end{align}
which we can rearrange to obtain
\begin{equation}
\delta \lambda = \frac{\int_{\Omega} \delta V \psi^2}{2\lambda \int_{\Omega} \psi^2 + \int_{\Gamma} \psi B'(\lambda) \psi}. \quad (35)
\end{equation}
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
\begin{equation}
\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}. \quad (36)
\end{equation}

5 Domain independence of the denominator

Now suppose that $\phi(x, \lambda)$ is the solution to a Dirichlet problem
\begin{align}
(\Delta + \lambda^2) \phi &= 0 \text{ on } \Omega \\
\phi &= f \text{ on } \Gamma = \partial \Omega \quad (37) \\
\frac{\partial \phi}{\partial n} &= B(\lambda) f \text{ on } \Gamma \quad (38)
\end{align}
where $B(\lambda)$ is an appropriate Dirichlet-to-Neumann map. Taking variations with respect to $\lambda$ gives us the problem
\begin{align}
(\Delta + \lambda^2) \delta \phi + 2\lambda \delta \lambda \phi &= 0 \text{ on } \Omega \\
\delta \phi &= 0 \text{ on } \Gamma \quad (40) \\
\frac{\partial \delta \phi}{\partial n} &= B(\lambda) \delta \phi + B'(\lambda) f \delta \lambda \quad (41) \\
&= B'(\lambda) f \delta \lambda \quad (42) \\
&= B'(\lambda) \phi \delta \lambda \text{ on } \Gamma. \quad (43)
\end{align}
Integrating the domain equation against $\phi$ now gives
\begin{equation}
\int_{\Omega} \phi (\Delta + \lambda^2) \delta \phi + 2\lambda \delta \lambda \int_{\Omega} \phi^2 = 0. \quad (45)
\end{equation}
If we integrate the first term by parts twice, we have

\[
\int_{\Omega} \phi (\Delta + \lambda^2) \delta \phi
\]

\[
= \int_{\Gamma} \left( \phi \frac{\partial \delta \phi}{\partial n} - \delta \phi \frac{\partial \phi}{\partial n} \right) + \int_{\Omega} \delta \phi (\Delta + \lambda^2) \phi
\]

\[
= \int_{\Gamma} \phi \frac{\partial \delta \phi}{\partial n}
\]

\[
= \delta \lambda \int_{\Gamma} \phi B'(\lambda) \phi.
\]

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 \(V\).