Spectral Element Solutions of the Schrödinger Equation in Unbounded Domains

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Abstract

We present a spectral element τ-method to compute the eigenvalues of the Schrödinger operator in unbounded domains with a locally piecewise smooth potential

$$\left\{-\frac{d^2}{dx^2} + V(x)\right\} u(x) = \lambda u(x) \ , \ V = V_{\pm} \text{ for } |x| > R \ .$$

The spectrum is composed of three types of solutions, bound states, scattering states and resonances. Bound states have L_2 eigenfunctions which belong to real negative eigenvalues and satisfy vanishing conditions at $\pm\infty$. Scattering states are generalized eigenfunctions corresponding to the real-valued continuous spectrum and they can be thought of as asymptotically left- or right-propagating waves. Resonances are the most interesting as they correspond to discrete eigenvalues which lie in the complex plane[1]. The resonant eigenfunctions are unbounded at $\pm\infty$ and are either inward or outward propagating depending on whether the imaginary part of the eigenvalue is positive or negative. The spectral density function, which is called the "density-of-states" in physics, is one of the most important quantities in quantum systems and is defined in terms of the bound and resonant state eigenvalues. Although the resonant eigenfunctions are non-physical the locations of their eigenvalues determine the reflection coefficient for the scattering states. This coefficient determines the electron current in practical quantum devices.

Traditionally, bound and resonant states have been computed using either cumbersome or inaccurate shooting techniques where the potential is approximated as piecewise constant[2], linear[3], or as a superposition of delta functions[4]. Recent advances in nanotechnology have enabled atomic-layer control in semiconductor devices which allows the experimentalist to tailor the potential profile and position the eigenvalues in a desired way. An important class of structures of this type are quantum well photo-detectors which rely on photon induced promotion of electrons from bound to scattering states[5], which carry current. The photon absorption probability depends strongly on the locations of the resonant eigenvalues and a reliable means of predicting the bound and resonant spectrum would allow for more efficient device design.

We demonstrate a rapidly converging multi-domain scheme to compute the bound states by using a rational mapping[6] which brings the left and right semi-infinite intervals onto the unit interval.

$$y_l = -2\frac{x_l + R}{x_l - R} + 1 \ , -\infty < x_l < -R, \qquad y_r = 2\frac{x_r - R}{x_r + R} - 1 \ , R < x_r < \infty$$

We obtain spectral convergence through this method, whereas the more standard approach of domain truncation grants only algebraic convergence due to inefficient distribution of nodes.

To compute the resonances we deform the coordinate system into the complex plane and take a contour along which the eigenfunction is asymptotically decaying. To create a perfectly matched layer (PML)[7, 8] which allows only outward-propagating solutions, the parametric curve is required to be at least C^2 continuous at the local interface. This does not alter the resonant spectrum since the coordinates are not a quantum mechanical observable. Two suitable coordinate deformations for the left and right PML are

$$z_l = x_l - ic(-x_l - R)^n, \ -\infty < x_l < -R, \qquad z_r = x_r + ic(x_r - R)^n, \ R < x_r < \infty$$

where $n \geq 2, \ c \in \mathbb{R}^+$. Both approaches can be combined to improve the convergence and allow the simultaneous computation of bound and resonant states. Generalization to higher dimensional problems with radial symmetry is straightforward, and will be presented as time permits.

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