THE COMPLEX-SCALING FOURIER-GRID HAMILTONIAN METHOD FOR RESONANCE STATE PROBLEMS

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We present a new complex scaling method for the study of resonance eigenstates without the use of basis set expansions. The procedure does not require the computation of potential matrix elements; the eigenvectors provide directly the values of the resonance wave functions at the space grid points. The simplicity, efficiency, and reliability of the method is illustrated by a case study of the tunneling in an anharmonic oscillator.

1. Introduction

It is well known that the resonance states characterized by complex energies correspond to poles of the resolvent operator \((E - \hat{H})^{-1}\) in the complex-energy plane of a non-physical higher Riemann sheet. Numerous techniques have been developed to compute these poles. One of the most powerful techniques popularized in the last decade is the method known as the complex scaling (coordinate-rotation, complex-coordinate, or dilatation) transformation\(^*\). As a result of the complex scaling transformation, \(r \rightarrow r e^{i\alpha}\), the eigenvalues corresponding to the bound states of \(\hat{H}\) stay invariant, while the branch cuts associated with the continuous spectrum of \(\hat{H}\) are rotated about their respective thresholds by an angle \(-2\alpha\) (assuming \(0 < \alpha < \pi/2\)), exposing the complex resonance states in appropriate strips of the complex energy plane. A crucial point from the computational point of view is that the eigenfunctions associated with the complex-scaling resonance wave functions are localized, i.e. square integrable. The square integrability led to the extension of well-established bound-state techniques to the determination of resonance energies (\(E_R\)) and widths (\(\Gamma\)) of metastable states.

\(^*\) For a recent review of the applications of complex-scaling methods to autoionization, predissociation, and multiphoton resonances, see ref. [3].

In this paper we discuss a complex scaling method without the use of basis set expansion. Because of its extreme simplicity in numerical implementation, the method has decisive advantages for problems where no appropriate basis set can be found or a large number of basis sets are required. The method makes use of the recent advancement of the calculation of bound state eigenvalues and eigenfunctions using the Fourier transform method [4]. A detailed description of the method is given in section 2. The utility of the method is illustrated in section 3 by a case study of the resonance eigenvalue problem in the tunneling in an anharmonic oscillator.

2. The complex-scaling Fourier-grid Hamiltonian method

Consider for simplicity a one-dimensional system described by the Hamiltonian

\[
\hat{H}(x) = \hat{T} + V(\hat{x}) ,
\]

where \(\hat{T} = p^2/2m\) is the kinetic energy operator. (Extension of the method to multi-channel problems will be described in a subsequent publication.) Under the complex scaling transformation, \(x \rightarrow x e^{i\alpha}\),

\[
\hat{H}(x) \rightarrow \hat{H}(\alpha) = \hat{H}(x e^{i\alpha}) = e^{-2i\alpha} \hat{T} + V(\hat{x} e^{i\alpha}) .
\]

It is known that the kinetic energy operator is best represented in the momentum representation. Since
\[ \langle k' | \hat{T} | k \rangle = (\hbar^2 k^2 / 2m) \delta(k - k') , \quad (3) \]

\( \hat{T} \) is diagonal in the \( |k\rangle \) representation. Here \(|k\rangle\) are the eigenfunctions of \( \hat{p} \), namely,

\[ \hat{P} |k\rangle = \hbar k |k\rangle , \]

and satisfy the orthonormal and completeness relationships, respectively,

\[ \langle k | k' \rangle = \delta(k - k') \quad (4) \]

and

\[ \tilde{f}_k = \int_{-\infty}^{\infty} |k\rangle \langle k| \, dk . \quad (5) \]

On the other hand, the potential energy term \( V(x) \) is diagonal in the coordinate representation,

\[ \langle x' | V(x) | x \rangle = V(x) \delta(x - x') . \quad (6) \]

Here \(|x\rangle\) are the eigenfunctions of the coordinate operator,

\[ \hat{x} |x\rangle = x |x\rangle , \quad (7) \]

and satisfy the relationships

\[ \langle x | x' \rangle = \delta(x - x') \quad (8) \]

and

\[ \tilde{f}_x = \int_{-\infty}^{\infty} |x\rangle \langle x| \, dx . \quad (9) \]

In the coordinate or Schrödinger representation, the Hamiltonian operator in eq. (2) becomes

\[ \langle x | \hat{H}(\alpha) | x' \rangle = e^{-2i\alpha} \langle x | \hat{T} | x' \rangle + V(x e^{i\alpha}) \delta(x - x') . \quad (10) \]

Using the identity operator, eq. (5), eq. (10) can be rewritten as

\[ \langle x | \hat{H}(\alpha) | x' \rangle = e^{-2i\alpha} \int_{-\infty}^{\infty} \langle k | k \rangle \, dk \]

\[ + V(x e^{i\alpha}) \delta(x - x') \]

\[ = (e^{-2i\alpha} / 2\pi) \int_{-\infty}^{\infty} e^{i(k - k') \delta(k - k')} \, dk \]

\[ + V(x e^{i\alpha}) \delta(x - x') , \quad (11) \]

where \( T_k = \hbar^2 k^2 / 2m \).

To discretize the continuous range of coordinate values \( x_i \), we adopt the Fourier grid method [4]. Here a uniform discrete spatial grid

\[ x_i = i\Delta x \quad (i = 1, 2, ..., N) \quad (12) \]

will be used where \( N \) is an odd integer number. The orthogonality condition (8) and the identity operator (9) may now be written as

\[ \Delta x \langle x_i | x_j \rangle = \delta_{ij} \quad (13) \]

and

\[ \tilde{f}_x = \sum_{i=1}^{N} |x_i\rangle \Delta x \langle x_i| \quad (14) \]

The grid size and spacing in coordinate space determines the reciprocal grid size in momentum space. Thus \( \Delta k = 2\pi / N\Delta x \). The central point in the momentum space grid is chosen to be \( k = 0 \), and the grid’s points are evenly distributed about zero.

The discretized version of the complex scaling operator (11) now has the following form (after some simplification and renormalization)

\[ H_{\alpha}(\alpha) = \langle x_i | \hat{H}(\alpha) | x_j \rangle \]

\[ = (2 e^{-2i\alpha} / N) \sum_{i=1}^{N} \cos[2\pi l(i-j)/N] T_i \]

\[ + V(x e^{i\alpha}) \phi_j , \quad (15) \]

where \( n = \frac{1}{2}(N-1) \), and \( T_i = (2/m)(\hbar nL/N\Delta x)^2 \). This leads to the following complex secular equations for the resonancel eigenvalues \( \wp_{\alpha} \):

\[ \sum_{j} [H_{\alpha}(\alpha) - \wp_{\alpha} \delta_{ij}] \psi_j^* = 0 , \quad (16) \]

where the eigenvectors \( \psi_j^* \) give directly the amplitude of the normalized solutions of the resonance wave functions \( \psi^* \) evaluated at the grid points \( x_j \), namely,

\[ \psi_j^* = \langle x_j | \psi^* \rangle = \psi^*(x_j e^{i\alpha}) . \quad (17) \]

3. Resonance eigenvalues in anharmonic oscillator – a case study

In this section, we consider the problem of the tunneling in the anharmonic oscillator
Table 1
Resonance energies \( (E_R - \frac{i}{2}I') \) (in au) for the anharmonic oscillator \( V(x) = \frac{1}{2}x^2 - 0.034x^3 \) computed using various theoretical methods

<table>
<thead>
<tr>
<th>( N )</th>
<th>CSB</th>
<th>CSFD</th>
<th>CSFGH</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.48567937 -0.286698 \times 10^{-2}i</td>
<td>0.4856786 -0.30 \times 10^{-2}i</td>
<td>0.48567937 -0.286698 \times 10^{-2}i</td>
</tr>
<tr>
<td>1</td>
<td>1.3915748 -0.134193 \times 10^{-2}i</td>
<td>1.391572 -0.13425 \times 10^{-2}i</td>
<td>1.3915748 -0.134193 \times 10^{-2}i</td>
</tr>
<tr>
<td>2</td>
<td>2.1321356 -0.687626 \times 10^{-1}i</td>
<td>2.13213 -0.68762 \times 10^{-1}i</td>
<td>2.1321356 -0.687626 \times 10^{-1}i</td>
</tr>
<tr>
<td>3</td>
<td>2.817874 -0.363974i</td>
<td>2.81786 -0.363976i</td>
<td>2.817874 -0.36397367i</td>
</tr>
<tr>
<td>4</td>
<td>3.586675 -0.777257i</td>
<td>3.58665 -0.77724i</td>
<td>3.58667470 -0.77725688i</td>
</tr>
</tbody>
</table>

\( a \) Vibrational quantum number. \( b \) Complex-scaling basis set expansion method (ref. [6]).
\( c \) Complex-scaling finite-difference method (ref. [7]). \( d \) Complex-scaling Fourier-grid Hamiltonian method (present work).

\[ V(x) = \frac{1}{2}x^2 - \lambda x^3, \quad (18) \]

which was used by Yaris et al. [5] and by Datta and Chu [6] to experiment with the complex scaling methods using basis set expansion procedures, and by Atabek and Lefebvre [7] using the finite difference method. Table 1 shows the comparison of the present calculation (CSFGH) with former studies. It is seen that the present method reproduces exactly the results obtained by the complex-scaling basis-set-expansion (CSB) method [6]. Further, the CSFGH method appears more accurate and far more efficient than the finite difference method. (In the current calculations, we use \( N = 61 \) space grid points, while in the finite difference method quoted in ref. [7], \( N = 4000. \))

The power of the present CSFGH method lies in its extreme simplicity — no potential matrix element calculation (which are usually the most time consuming and difficult part in the basis set expansion method) are required. Further the eigenvectors provide directly the values of the resonance wave functions at the grid points. It appears that the CSFGH method is most valuable for highly excited problems where the basis set expansion methods face the challenge. Extension of this technique to multi-channel problems such as ac and dc Stark resonance of Rydberg states and vibrational–rotational predissocia-

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References