Conjecture on the Interlacing of Zeros in Complex
Sturm-Liouville Problems

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Abstract

The zeros of the eigenfunctions of self-adjoint Sturm-Liouville eigenvalue problems interlace. For these problems interlacing is crucial for completeness. For the complex Sturm-Liouville problem associated with the Schrödinger equation for a non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian, completeness and interlacing of zeros have never been examined. This paper reports a numerical study of the Sturm-Liouville problems for three complex potentials, the large-$N$ limit of a $-(ix)^N$ potential, a quasi-exactly-solvable $-x^4$ potential, and an $ix^3$ potential. In all cases the complex zeros of the eigenfunctions exhibit a similar pattern of interlacing and it is conjectured that this pattern is universal. Understanding this pattern could provide insight into whether the eigenfunctions of complex Sturm-Liouville problems form a complete set.
I. INTRODUCTION

The spectra of many classes of non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians are real and positive [1–13]. It is believed that the positivity of the spectra is a consequence of $\mathcal{PT}$ symmetry. Examples of heavily studied $\mathcal{PT}$-symmetric Hamiltonians are [1,2]

$$H = p^2 - (ix)^N \quad (N \geq 2) \quad (1.1)$$

and [3]

$$H = p^2 - x^4 + 2iax^3 + (a^2 - 2b)x^2 + 2i(ab - J)x \quad (J \ \text{integer}, \ a^2 + 4b > K_{\text{critical}}), \quad (1.2)$$

where $K_{\text{critical}}$ grows with increasing $J$. For Hamiltonians like those in (1.1) and (1.2) the Schrödinger equations for the $k$th eigenfunction,

$$H \Psi_k(x) = E_k \Psi_k(x), \quad (1.3)$$

involve a complex potential and may require $x$ to be complex for the boundary conditions to be defined properly [14]. Thus, the Schrödinger eigenvalue problems may be regarded as analytic extensions of Sturm-Liouville problems into the complex plane.

The eigenfunctions of a conventional self-adjoint Sturm-Liouville problem are complete. Completeness is the statement that a given function can be represented as a linear superposition of the eigenfunctions:

$$f(x) = \sum_n a_n \Psi_n(x). \quad (1.4)$$

It is necessary for the zeros of the eigenfunctions in the complete set to become dense on the interval in which the Sturm-Liouville problem is defined. If the zeros did not become dense, it would be impossible to represent a rapidly varying function [15,16]. For conventional Sturm-Liouville problems one can prove that the zeros of successive eigenfunctions interlace, and this interlacing of the zeros ensures that the zeros become dense [15].

A major open mathematical question for $\mathcal{PT}$-symmetric Hamiltonians is whether the eigenfunctions form a complete set. If the zeros of the eigenfunctions of complex Sturm-Liouville eigenvalue problems exhibit the property of interlacing, this provides heuristic
evidence that the eigenfunctions might be complete. A proof of completeness would require that we identify the space in which they are complete, and we do not yet know how to do this. Nevertheless, if we can understand the distribution of the zeros of the eigenfunctions, we gain some insight into the question of completeness for eigenfunctions of $\mathcal{PT}$-symmetric Sturm-Liouville problems.

II. SOME EXAMPLES OF DISTRIBUTIONS OF ZEROS

We have studied three different complex $\mathcal{PT}$-symmetric Hamiltonians. We find that in every case the qualitative features of the distribution in the complex plane of the zeros of the eigenfunctions are very similar: We observe a shifted interlacing of zeros. We believe that this pattern of zeros is universal.

**Example 1: Large-$N$ limit of the $-(ix)^N$ potential.** The large-$N$ limit of a $-(ix)^N$ potential is exactly solvable $[5]$. In Fig. 1 the zeros of the 14th and 15th eigenfunctions are plotted and clearly exhibit a form of interlacing in the complex plane. For convenience, we have scaled the zeros by dividing by the magnitude of the turning points; we have then performed a linear transformation to fix the turning points at $\pm 1$. The appropriate scaling is

$$z = (xE^{-1/N} + i)N/\pi.$$ \hspace{1cm} (2.1)

As shown in Fig. 2, the zeros of the first 15 eigenfunctions interlace and appear to become dense in a narrow region surrounding an arch-shaped contour in the complex plane. This contour is the Stokes’ line that joins the turning points; that is, it is the path along which the phase in the WKB quantization condition is purely real (and thus the quantum-mechanical wave function is purely oscillatory) $[1]$. (It is interesting that this WKB path differs from the path that a classical particle follows in the complex plane as it oscillates between the turning points. The path that a classical particle follows is an inverted arch-shaped contour between the same two turning points. $[2]$)
Example 2: Quasi-exactly-solvable \(-x^4\) potential. Next, consider the quasi-exactly-solvable potential in (1.2) with \(a = 10\) and \(b = 2\). The eigenfunctions of the Schrödinger equation have the form of an exponential multiplied by a polynomial. The zeros of this polynomial are easy to calculate numerically. For a given \(J\) the polynomials in the eigenfunctions all have the same degree and, as a result, all of the eigenfunctions have the same number of zeros. However, for the \(k\)th wave function, \(J - k\) zeros lie along the branch cut on the positive imaginary axis, and we consider these zeros to be irrelevant. For values of \(J\) ranging from 1 to 21, the qualitative behavior is always the same. In Fig. 3 the results for \(J = 21\) are plotted and the relevant zeros again lie along the WKB paths in the complex plane. In this case the zeros are not contained in as narrow a region of the complex plane as for the \(-(ix)^N\) potential because the zeros have not been scaled as in Fig. 2. The zeros have an imaginary part that becomes more negative as \(k\) increases and exhibit the complex version of interlacing.

In Fig. 4 the zeros are scaled so that \(z = x/|x_{TP}|\), where \(|x_{TP}|\) are the magnitudes of the classical turning points. (The classical turning points are the roots of \(-x^4 + 20ix^3 + 96x^2 - 2ix = E.\)) The scaled zeros lie in a more compact region in the complex-z plane than the zeros in Fig. 3. We believe the zeros become dense in this region. Notice that this arch-shaped region is broader than the corresponding region in Fig. 2 because the turning points do not all lie along the same polar angle; therefore, the scaling fixes the magnitudes but not the positions of the turning points. Potentials with various values of \(a\) and \(b\) were also investigated and similar results were obtained.

Example 3: \(ix^3\) potential We obtain an \(ix^3\) potential when we set \(N = 3\) in (1.1). Using Runge-Kutta techniques in the complex plane, we have plotted the level curves of the real and imaginary parts of the complex eigenfunctions. By finding the intersections of these level curves, we have determined the zeros of the eigenfunctions numerically. These zeros, which are shown in Fig. 5, lie along the Stokes’ lines of the WKB approximation. Again, the zeros exhibit the complex version of interlacing. They have an imaginary part that
decreases as \( k \) increases. In Fig. 6 the zeros are scaled by \( z = x/|x_{TP}| = xE^{-1/3} \), which fixes the magnitudes and positions of the turning points. This plot suggests that after the scaling the zeros become dense in the complex-\( z \) plane. Once again, this plot suggests that the distribution of zeros in the complex plane is a universal property of complex Sturm-Liouville eigenvalue problems associated with \( \mathcal{PT} \)-symmetric Hamiltonians.

**Statement of the Conjecture**

From our studies we observe that the unscaled zeros of the complex eigenfunctions do not become dense on a contour or in a narrow region of the complex-\( x \) plane. In particular, for the \( ix^3 \) potential WKB theory predicts that \( E_k \sim Ck^{6/5} \) \((k \to \infty)\), where \( C \) is a constant. Thus, the turning points behave like \( x_{TP} \sim (-iC)^{1/3}k^{2/5} \) \((k \to \infty)\) and

\[
\frac{dx_{TP}}{dk} \sim \frac{2}{5}(-iC)^{1/3}k^{-3/5} \quad (k \to \infty).
\]  

(2.2)

Using Richardson extrapolation we have verified that the distance between zeros along the imaginary axis exhibits this \( k \)-dependence. Consequently, the distance from the contour along which the zeros of \( \Psi_1 \) lie to the contour along which the zeros of \( \Psi_k \) for large \( k \) lie is given by \( \sum_{k=0}^{\infty} k^{-3/5} \) which is infinitely far away.

We have scaled the zeros by fixing the magnitudes of the turning points relative to a unit length. After this scaling is performed, the zeros appear to become dense in a narrow arch-shaped region in the scaled complex plane. If the zeros do become dense in this narrow region and exhibit the shifted complex version of interlacing, we conjecture that this behavior suggests that the eigenfunctions are complete in the scaled complex plane. Since we do not know what space within which to define completeness, we are unable to give a rigorous proof.

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FIG. 1. Zeros of the 14th and 15th eigenfunctions, $\Psi_{14}(x)$ and $\Psi_{15}(x)$, of the $-(ix)^N$ potential in the large-$N$ limit. The plot shows the $z$-plane where the turning points have all been scaled to $-1$ and $1$ as in (2.1). The zeros lie in a small arch-shaped region in the complex plane. For any two zeros of $\Psi_{15}(z)$, a zero of $\Psi_{14}(z)$ lies between them along the arch-shaped region. This is a complex version of interlacing.
FIG. 2. Zeros for the first 15 eigenfunctions of the $-(ix)^N$ potential in the large-$N$ limit. The plot shows the $z$-plane where the turning points have all been scaled to $-1$ and $1$ as in (2.1). The complex version of interlacing in Fig. 1 is again evident in this plot, but this plot also suggests that the zeros are becoming dense in a small region in the complex-$z$ plane.
FIG. 3. Zeros for the 21 exactly solvable eigenfunctions of the quasi-exactly-solvable $-x^4$ potential in (1.2). The zeros lie in a small arch-shaped region in the complex-$x$ plane and exhibit a complex version of interlacing. The zeros do not become dense in a region of the complex-$x$ plane because the zeros lie on the Stokes’ line of the wave function (the curve along which the wave function is oscillatory). These curves are different for each eigenfunction; the curves move downward as the energy increases and there is no limiting curve.
FIG. 4. Zeros for the 21 exactly solvable eigenfunctions of the quasi-exactly-solvable $-x^4$ potential (1.2) with the magnitudes of the turning points fixed. The plot shows the complex-$z$ plane in which the magnitudes of the turning points are fixed to unit length. In the $z$ plane the zeros lie in a much narrower arch-shaped region than in Fig. 3. Once again, the zeros exhibit a complex version of interlacing, and now, we believe they become dense in a narrow region of the scaled complex plane.
FIG. 5. Zeros of the first six eigenfunctions of the $ix^3$ potential. These zeros lie in a small arch-shaped region in the complex plane and exhibit a complex version of interlacing. The zeros do not become dense in a region of the complex plane because, as in Fig. 3, the zeros lie on a sequence of curves that move downward with increasing energy and remain well separated.
FIG. 6. Zeros for the first six eigenfunctions of the $ix^3$ potential with the turning points fixed. The plot is done in the complex-$z$ plane where the magnitudes of the turning points are fixed to unit length. As a result, the zeros lie in a narrower arch-shaped region in the complex plane than in Fig. 5. The zeros exhibit a complex version of interlacing and we believe they become dense in the scaled complex-$z$ plane.