Non-Hermitian Particle in a Box with Altered Boundary Conditions

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Introduction

A fundamental principle of quantum mechanics is that all observables must be represented by hermitian operators. Recently Carl Bender showed that it is possible to relax this assumption under suitable conditions. Non-hermitian quantum mechanics allows us to consider new Hamiltonians that are not allowed by conventional quantum mechanics. In this paper, we will discuss how non-hermitian quantum mechanics permits new boundary conditions on electron wavefunctions that are not allowed in conventional quantum mechanics. Boundary conditions play a key role in determining the properties of a class of solids called topological insulators such as the existence of electronic states bound to the surface of the solid. Our results may therefore have relevance to the physics of topological insulators. These systems have PT-symmetry, which means that the systems are the same under parity (spatial reflection) and time reversal.

Motivation

Quantum mechanics has not been altered since the theory was first set, so the goal is to see if it is possible to alter the theory in such a way to allow more systems to be analyzed. There are four major postulates in quantum mechanics, which are:

- The wavefunctions are normalized.
- The wavefunction satisfies the Schrödinger equation.
- The Hamiltonian is Hermitian.

The last condition is strictly mathematical, and could be showed to be altered to having PT-symmetry.

2-Level System

An example of a system that is PT-symmetric is known as the two-level system. This is a very simple system, where the Hamiltonian of the system is considered to be a 2 by 2 matrix. The general form of a PT symmetric Hamiltonian is given below. This system will obey all the requirements of a PT quantum mechanical system, which means:

- The energy eigenvalues are real.
- The Hamiltonian is PT-symmetric.
- The Hamiltonian is PT self-adjoint, meaning that the inner products are equivalent or in other words, $(\langle \phi | H | \psi \rangle)_{PT} = (\langle H | \phi | \psi \rangle)_{PT}$

\[
\begin{pmatrix}
 a & ib \\
 ib & c
\end{pmatrix}
\]

PT Symmetry

In Hermitian quantum mechanics, it can be shown that the boundary conditions for a particle in a box can be generalized to the equation shown below, where $\psi(x)$ is the wavefunction of the boundary, and $\lambda$ is a real parameter defined as the penetration depth.

\[
\psi(x) - \frac{d}{dx} \psi(x) = 0
\]

Since the requirement that the parameter be real is based purely on the requirement that the Hamiltonian be Hermitian, it is possible to break this condition using PT symmetry. Using PT symmetry, one obtains the condition on $\lambda$ shown below:

\[
\lambda = \lambda_1 + i\lambda_2 \quad \text{at } x=0
\]
\[
\lambda = -\lambda_1 + i\lambda_2 \quad \text{at } x=L
\]

Note: That in this situation, the penetration depth is not real, but complex, and that the value of this parameter depends on which boundary one is evaluating the wavefunction at.

PT Self-Adjoint

A system is considered to be PT Self-Adjoint if the inner product with the Hamiltonian acting on one wavefunction produces the same eigenvalues if the Hamiltonian is acted upon by another wavefunction in the inner product. For the particle in a box, this condition results in needing to evaluate the following inner product:

\[
\left( \frac{d}{dx} \phi \right)_{PT} = \left( \phi \frac{d}{dx} \right)_{PT}
\]

The following condition can be evaluated, and upon evaluating, it is possible to show that in order for the particle in a box system to be PT self-adjoint, the following condition must hold true:

\[
\Phi^\dagger (L-x)\psi(x) \frac{d}{dx} \phi(L-x)\psi(x) = 0
\]

The previous condition is satisfied by the above boundary conditions. Since the condition is satisfied, the particle in a box with the above altered boundary conditions is PT self-adjoint.

Eigenvalues

If $\lambda$ is to be considered completely imaginary, which obviously disobeys hermiticity, it is possible to find wavefunctions that satisfy both the Hamiltonian and the boundary conditions. These wavefunctions are different than those found for the typical particle in a box, but interestingly enough, the eigenvalues of the energy work out to be the same in both situations. These energy eigenvalues are shown below.

\[
E = \frac{k^2}{2}, k = \frac{\pi n}{L}, n = 0, 1, 2, ...
\]

Also, another interesting fact is that if $\lambda$ is allowed to be complex, but still satisfy the boundary conditions, in other words $\lambda_1$ and $\lambda_2$ are both non-zero, it is still possible to find real energy eigenvalues that correspond to wavefunctions that satisfy the Hamiltonian and the boundary conditions. The eigenvalues found in this situation are given below to first order.

\[
E = \frac{k^2}{2}, k = \frac{\pi n}{L}, n = 0, 1, 2, ...
\]

Where $\Delta k$ is the change in the $k$ values. These show that the system we created has broken PT symmetry for all values of $\lambda_1$ and $\lambda_2$ and thus have a completely new non-hermitian quantum mechanical system.

Conclusions

The work shows that this new system satisfies the requirements of a PT quantum system, the Hamiltonian with the altered boundary conditions have PT symmetry, the boundary conditions are PT self-adjoint, and the eigenvalues are real. This work demonstrates the new systems that can be analyzed through the use of non-hermitian quantum mechanics and allows the boundary conditions to be altered creating a new family of possible Hamiltonians that fit into PT quantum mechanics.

Future Work

Since the project deals with altered boundary conditions, it is feasible that this new system will help to describe phenomena that mainly involve interactions on the bound states. This would be possible, because our work shows that using altered boundary conditions and PT quantum mechanics, the resulting system has real eigenvalues.

References