An Analytical Approach for the Energy Eigenvalues Solution in a Double-Well Potential
Collaborators

- Sree Ram Valluri (University of Western Ontario)
- Ken Roberts (University of Western Ontario)
- Pranawa Deshmukh (Indian Institute of Technology, Tirupati)
- Rob Scott (University of Brest, France)
- Harsh Narola (Indian Institute of Technology, Tirupati)
- Shantanu Basu (University of Western Ontario)
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Introduction

- The one dimensional finite square well potential (FWSP) is a widely studied topic in introductory quantum mechanics.
- The quantum finite square well (FSW) problem is usually solved as a set of transcendental equations.
- An analytical solution for this problem does not exist, however, exact solutions based on contour integration are of great interest.

A new approach to this problem is based on the Lambert W function, which has triggered our interest in the quantum double square well potential [DSWP].
The DSWP problem is of great interest in both physics and quantum chemistry. An example of an application of the DSWP in both of these fields is with the Tunneling of the Nitrogen Atom in the Ammonia Molecule through a classically forbidden region to acquire stability.

Charles H. Townes employed this model in his Nobel prize (physics 1964) winning work on the Ammonia Maser.
Our Approach

Process

- Although the DSWP does not need to be symmetrical, knowing the solutions for a symmetrical DWSP may provide some useful insight in solving the asymmetrical DSWP.

Our Model Potential of choice: a Symmetric Double Square Well
The Context of the symmetric DSWP problem

Given the SWP of the three regions, the reduced wave function \( \psi(x) \) has values in the three regions given by:

\[
\psi_1(x) = A_1 e^{-i\alpha x} + A_2 e^{i\alpha} \quad (1)
\]
\[
\psi_2(x) = B_1 e^{-\beta x} + B_2 e^{\beta x} \quad (2)
\]
\[
\psi_3(x) = C_1 e^{-i\alpha x} + C_2 e^{i\alpha x} \quad (3)
\]

\[
\alpha^2 = \frac{2m(V_0 + E)}{\hbar^2} = \frac{2m}{\hbar^2} (V_0 - |E|) \quad (4) \quad \alpha > 0
\]
\[
\beta^2 = \frac{-2mE}{\hbar^2} = \left( \frac{2m}{\hbar^2} |E| \right) \quad (5) \quad \beta > 0
\]

\[
-V_0 \leq E < 0
\]

\( m \) is the mass of the particle bound in the square well
\( \hbar \) is the reduced Planck's constant

\( \Psi(x) \) is zero outside of \(-L < x < L\)

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**Methodology**

Fig. 1 1D infinite square well with a finite barrier
The Context of the symmetric DSWP problem

We aim to determine the values of E for which the reduced wave function $\psi(x)$ is smooth for all of $x$ satisfying $-L < x < L$ and $\psi(L) = \psi(-L) = 0$

$\psi(x)$ satisfies the time-independent Schrodinger equation:

$$-\frac{\hbar^2}{2m}\psi''(x) = -V(x)\psi(x) + E\psi(x)$$  \hspace{1cm} (6)

Fig. 1 1D infinite square well with finite barrier
The Structural and Radial Equations for the DSWP

We define
\[ u = \beta a \]
\[ v = \alpha a \]
\[ f = \frac{(L - a)}{a} \]

We also define
\[ R^2 = (\alpha^2 + \beta^2)a^2 = \frac{a^2V_02m}{h^2} \]

The \( \psi(x) \) solutions are either even or odd functions

\( \epsilon = +1 \) \[ \text{[For even } \psi(x)\text{]} \]
\( \epsilon = -1 \) \[ \text{[For odd } \psi(x)\text{]} \]

\( u \) and \( v \) are real.

\( R \) is a real dimensionless quantity, called the strength of the FSW

The DSWP reduces to finding the solutions of two simultaneous equations

The Structural Equation:
\[ e^{i2f\nu} = \frac{-(iv - u)e^u + \epsilon(iv - u)e^{-u}}{(iv + u)e^u + \epsilon(iv - u)e^{-u}} \]

and

The Radial Equation:
\[ u^2 + v^2 = R^2 \]

These two equations are to be solved in order to determine the bound energy levels of the symmetric DSWP.
Analysis of the Structural Equation

Case #1: $Re\ e^{2iv} = 0$

When $\epsilon = 1$

$$(f - 1)v \tan(f - 1)v = (f - 1)u \tanh u$$

When $\epsilon = -1$

$$(f - 1)v \tan(f - 1)v = (f - 1)u \coth u$$

Case #2: $Im\ e^{2iv} = 0$

When $\epsilon = 1$

$$(f - 1)v \cot(f - 1)v = -(f - 1)u \tanh u$$

When $\epsilon = -1$

$$(f - 1)v \cot(f - 1)v = -(f - 1)u \coth u$$

Question to be answered: Can one call this the ‘Generalized Curves of Hippias’?
The Geometric Approach– Single finite square well

A comparable approach can be derived from the problem when there is only one well.

For the single finite square well, we also get structural and radial equations.

We define

\[ \xi = \alpha a \]
\[ \eta = \beta a \]

We also define

\[ \xi \cot \xi = -\eta \quad \text{(For odd states)} \]
\[ \xi \tan \xi = \eta \quad \text{(For even states)} \]

Note that \( \xi \) and \( \eta \) must be positive, such that

\[ \xi^2 + \eta^2 = \gamma^2 \]

Note that \( \xi = \nu \), \( \eta = u \), \( \gamma = R \).
The Geometric Approach

The Geometric approach to the single FSWP involves the mapping of the Lambert W function in both the W and Z-plane.

Figure 2. Lambert lines in the W-plane ($u$ is along the horizontal axis and $v$ is along the vertical axis)

Figure 3. Lambert lines in the Z-plane

The intersection points of the lines in the W-plane correspond with points in the Z-plane.
The Geometric Approach

- We seek an analytical solution to the DSWP using the Lambert W technique that uses a smooth mapping.
- We ask the question: How would the scattering be represented, not in experiment space, but in solution space?
- Analytical ideas, as well as geometric ideas and visualization, should complement numerical computer calculations.
The Geometric Approach - DSWP

For the DSWP, we map the radial equation $u^2 + v^2 = R^2$ in both the W and Z-plane.

**Fig 4.** Radial equation in W-plane.
- Blue solid dots = even solutions
- Red hollow diamonds = odd solutions.

**Fig 5.** Radial equation in Z-plane.
- Blue solid dots = even solutions
- Red hollow diamonds = odd solutions.
Typical scenario of plane wave incidence on a hollow cylindrical potential:

**Idea:**
- We apply the analysis to the scattering of electrons off a hollow cylindrical potential, such as a transverse section of a nanotube.
- Initially presented by Sudhir and Deshmukh in 2010.

**Aim:**
- Represent the solution as an intersection of surfaces in three dimensions, even though it is a two-dimensional physical coordinate space.
Idea: Possible realization of Levinson’s Theorem by Manangath, Auddy, and Deshmukh (IIT, Chenai, April 2013)

Fig 8. Delta as a function of $U$

Fig 9. Real Lambert lines in the W-plane

The asymptotic spacing of the real Lambert lines illustrates the connection to Levinson’s Theorem.


The Geometric Approach—single finite square well

The solutions for the bound energies is obtained using two different mapping of geometric structures between Z-plane and W-plane.

**Mapping one:**

1. Start with a circle of a fixed radius $R$ in W-plane.
2. Map each of the four axes in the Z-plane to the W-plane via the inverse [Lambert W function] of the map $we^w = z$.
3. The lines are Lambert lines, which represent the branches of the Lambert W function.
4. The intersections/points are all the possible solutions of a FSW of strength $R$.

The intersection points are the solutions for the allowed energies for the FSWP
Mapping two:

1. Start with a circle of radius $R$ in the $W$-plane.
2. Map the $W$-plane to the $Z$-plane using $we^w = z$, which will give a closed curve that loops around the origin several times.
3. The intersections/points of the four axes are all the possible solutions of a FSW of strength $R$.

The intersection points are the solutions for the allowed energies for the FSWP.

Figure 3. Lambert lines in the $Z$-plane
The Geometric Approach - DSWP

For the DSWP, we graph the radial equation $u^2 + v^2 = R^2$ in both the W and Z-plane.

A closer view of quadrant 1 of z-plane graph.
We consider geometric arrangements to make the physics work

**Idea #2:**

- We transform the scattering problem by a conformal map to make the incoming particle occupy the entire left half plane, and the outgoing particle occupy the entire right half plane.

**Benefit:** There is symmetry of the problem, when reflected about imaginary axis.