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

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Talk Outline

1. Introduction
2. Application of the DSWP problem
3. Our approach
4. The context of the DSWP problem
5. The Geometric Approach
6. Looking forward- further possibilities
7. References

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].

Application of the DSWP Problem

- 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.

Charles H. Townes
(1915-2015)

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

Methodology

The Context of the symmetric DSWP problem

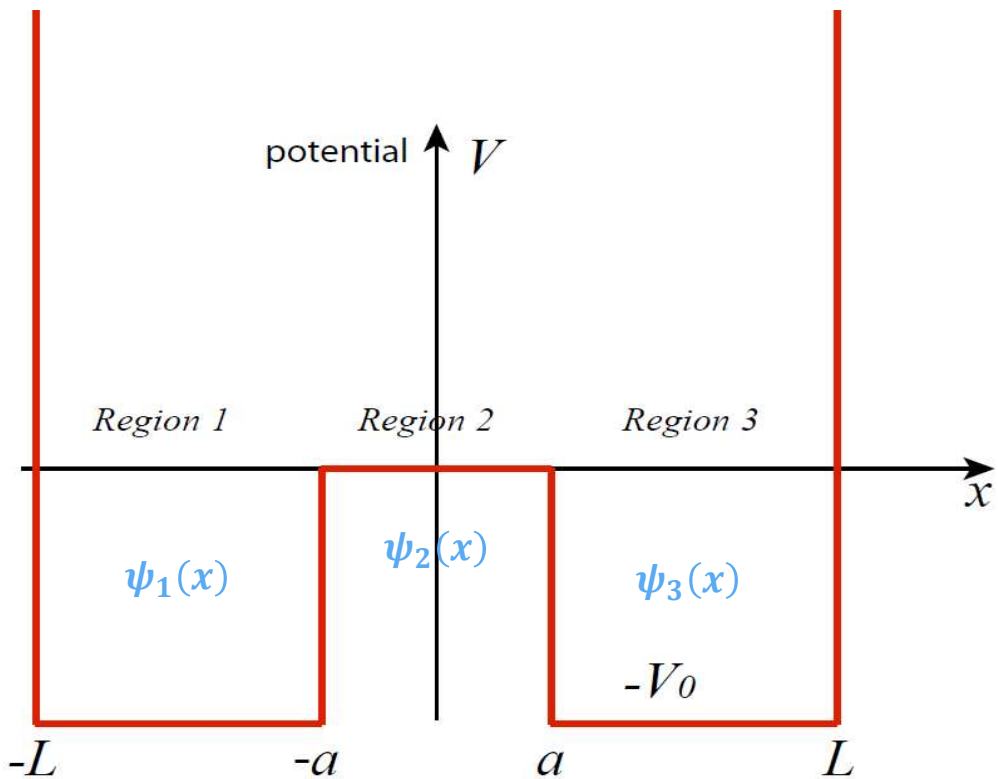


Fig. 1 1D infinite square well with a finite barrier

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

$$\psi_1(x) = A_1 e^{-i\alpha x} + A_2 e^{i\alpha} \qquad (1)$$

$$\psi_2(x) = B_1 e^{-\beta x} + B_2 e^{\beta x} \qquad (2)$$

$$\psi_3(x) = C_1 e^{-i\alpha x} + C_2 e^{i\alpha x} \qquad (3)$$

$$\alpha^2 = \frac{2m(V_0 + E)}{\hbar^2} = \frac{2m}{\hbar^2}(V_0 - |E|) \qquad (4) \qquad \alpha > 0$$

$$\beta^2 = \frac{-2mE}{\hbar^2} = \left(\frac{2m}{\hbar^2}|E|\right) \qquad (5) \qquad \beta > 0$$

$$-V_0 \leq E < 0$$

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 $-L < x < L$

Methodology

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:

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

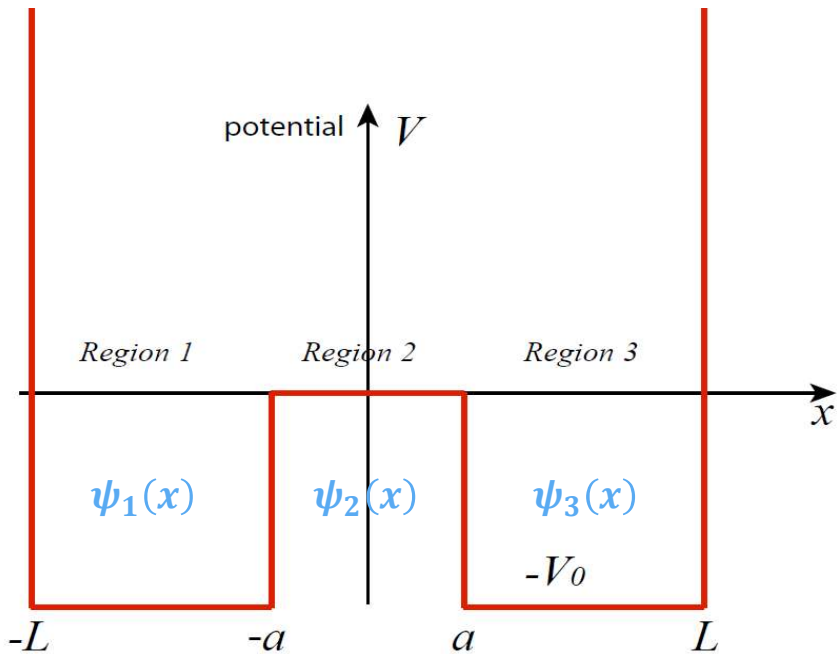


Fig. 1 1D infinite square well with finite barrier

The Structural and Radial Equations for the DSWP

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

We define

$$u = \beta a$$

$$v = \alpha a$$

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

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

$$f = \frac{(L-a)}{a}$$

We also define

$$R^2 = (\alpha^2 + \beta^2)a^2 = \frac{a^2 V_0 2m}{\hbar^2}$$

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:

$$e^{i2fv} = \frac{-(iv-u)e^{u} + \epsilon(iv-u)e^{-u}}{(iv+u)e^{u} + \epsilon(iv-u)e^{-u}}$$

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: $Re\ \mathrm{e}^{2\mathrm{iv}} = 0$

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

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 ξ and η must be positive, such that

$$\boxed{\xi^2 + \eta^2 = \gamma^2}$$

Note that $\xi = v \qquad \eta = u \qquad \gamma = R$

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.

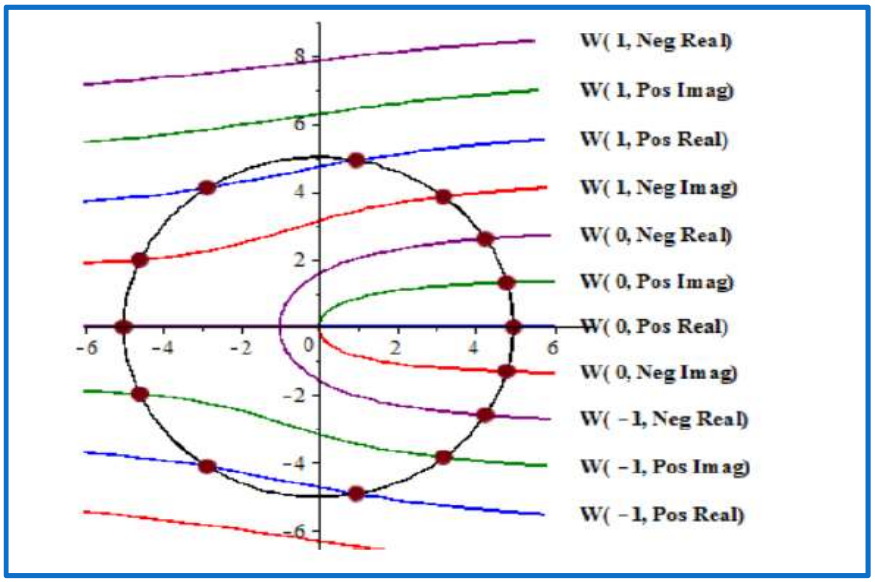


Figure 2. Lambert lines in the W-plane (u is along the horizontal axis and v is along the vertical axis)

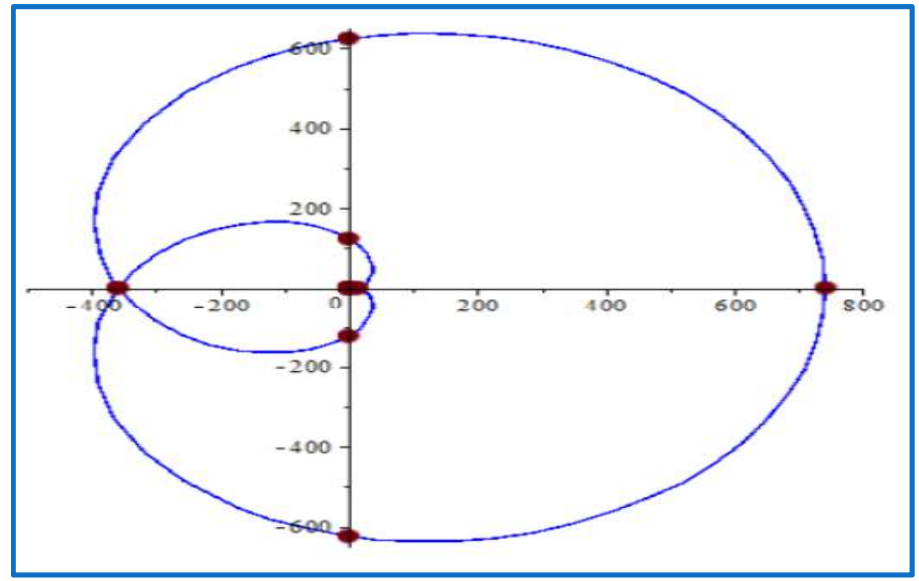


Figure 3. Lambert lines in the Z-plane

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.

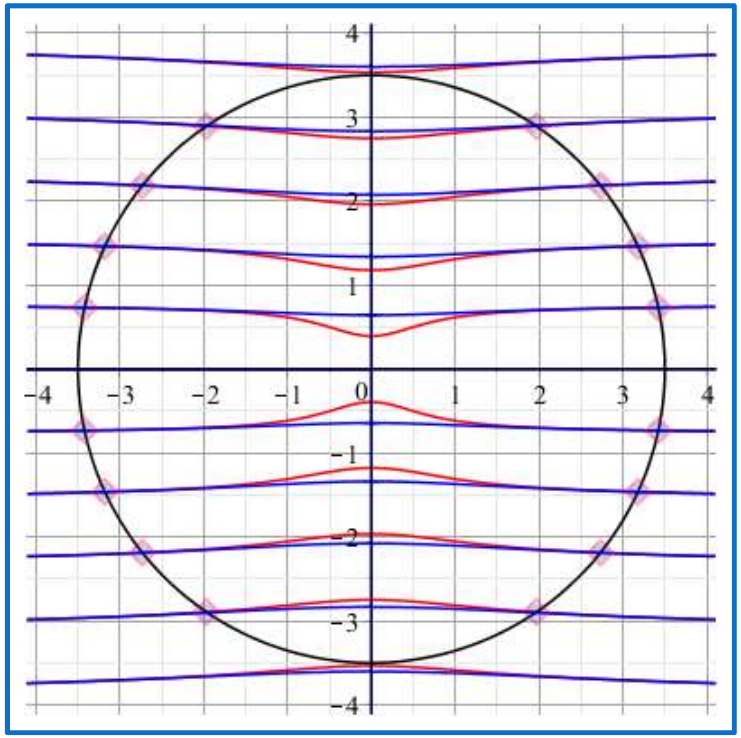


Fig 4. Radial equation in W-plane.
- Blue solid dots = even solutions
- Red hollow diamonds = odd solutions.

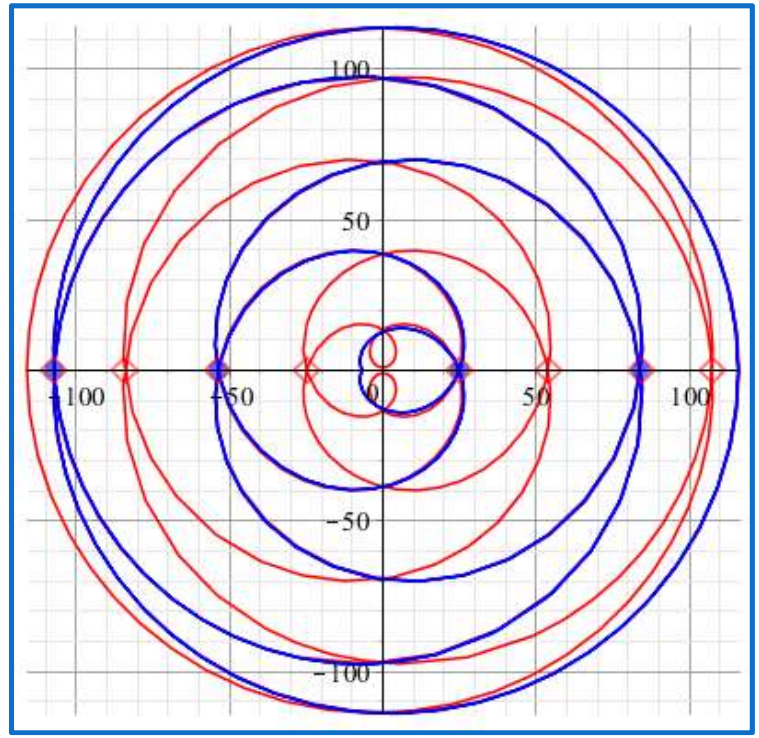


Fig 5. Radial equation in Z-plane.
- Blue solid dots = even solutions
- Red hollow diamonds = odd solutions.

Looking Forward– Further Possibilities

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.

Typical scenario of plane wave incidence on a hollow cylindrical potential:

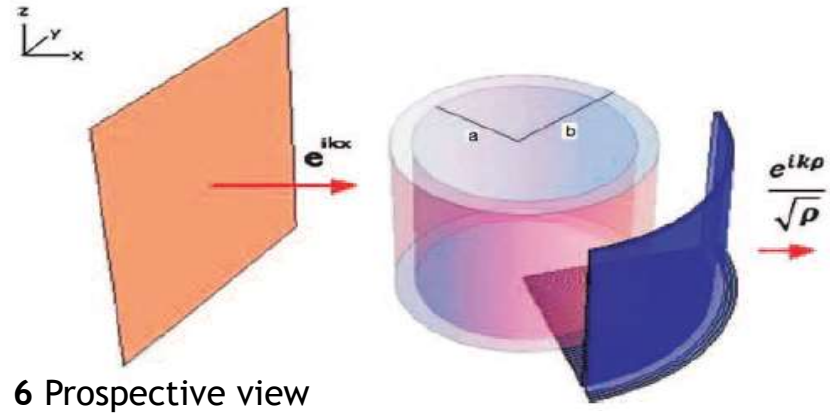


Fig. 6 Prospective view

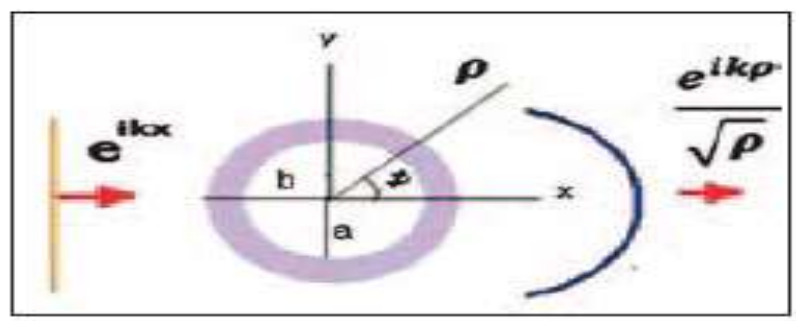


Fig. 7 Plane view

(Sudhir and Deshmukh 2010)

Idea : Possible realization of Levinson's Theorem by Manangath, Auddy, and Deshmukh (IIT, Chenai, April 2013)

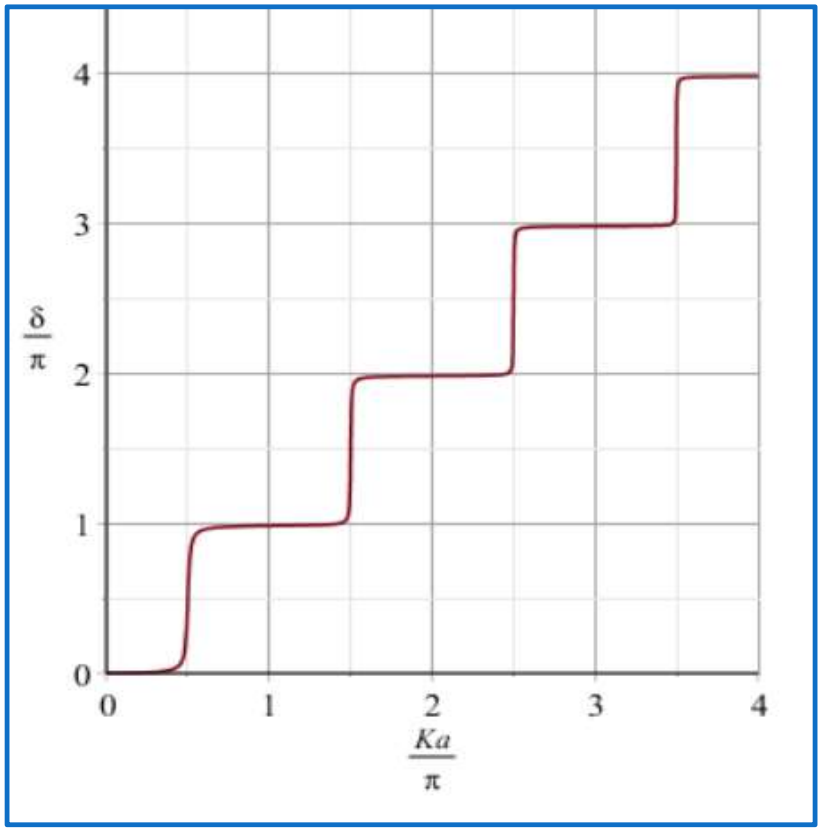


Fig 8. Delta as a function of U

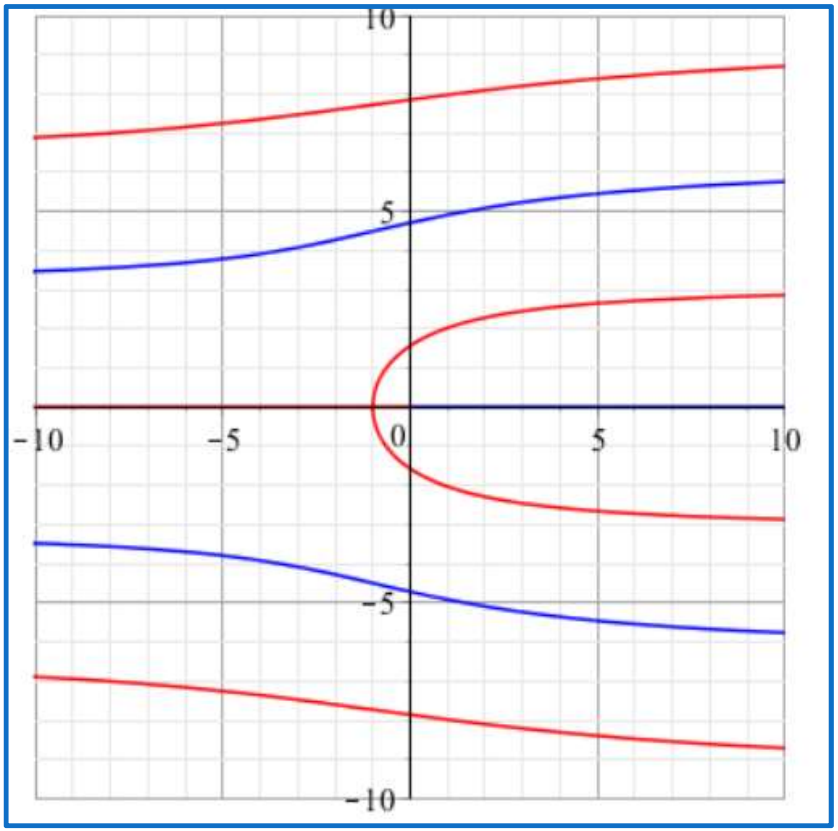


Fig 9. Real Lambert lines in the W-plane

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

References

K. Roberts and S.R Valluri. *Can J. Phys*. 95,105 (**2017**).

V. Sudhir and P.C. Deshmukh. *J. Comput. Theor. Nanosci*. 7, 10 (**2010**).

V. Sudhir and P.C. Deshmukh. J. Comput. Theor. Nanosci. 8, 1 (**2011**).

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.

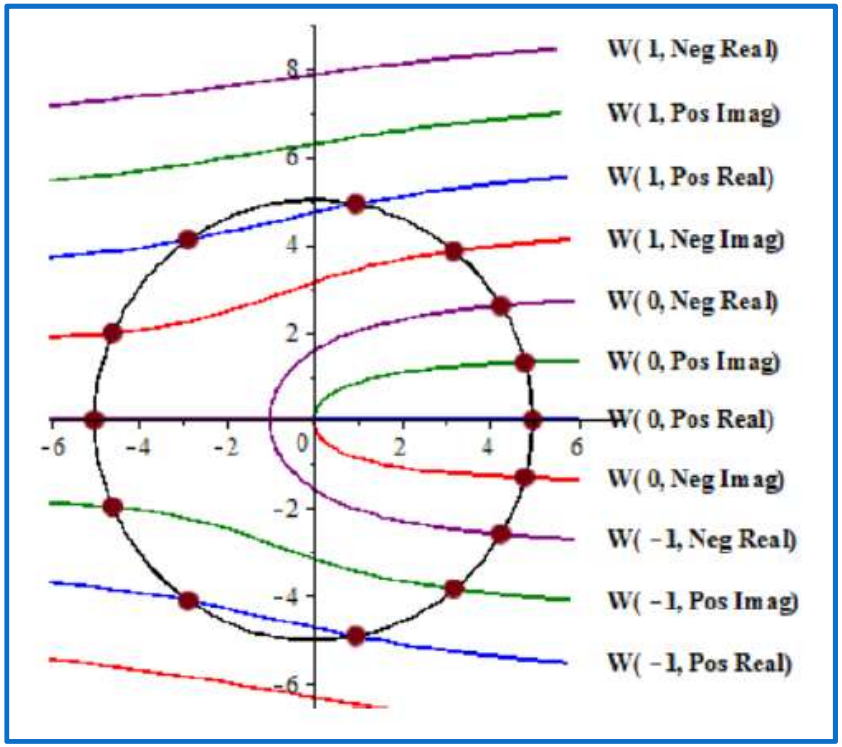


Figure 2. Lambert lines in the W-plane

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

The Geometric Approach- single finite square well

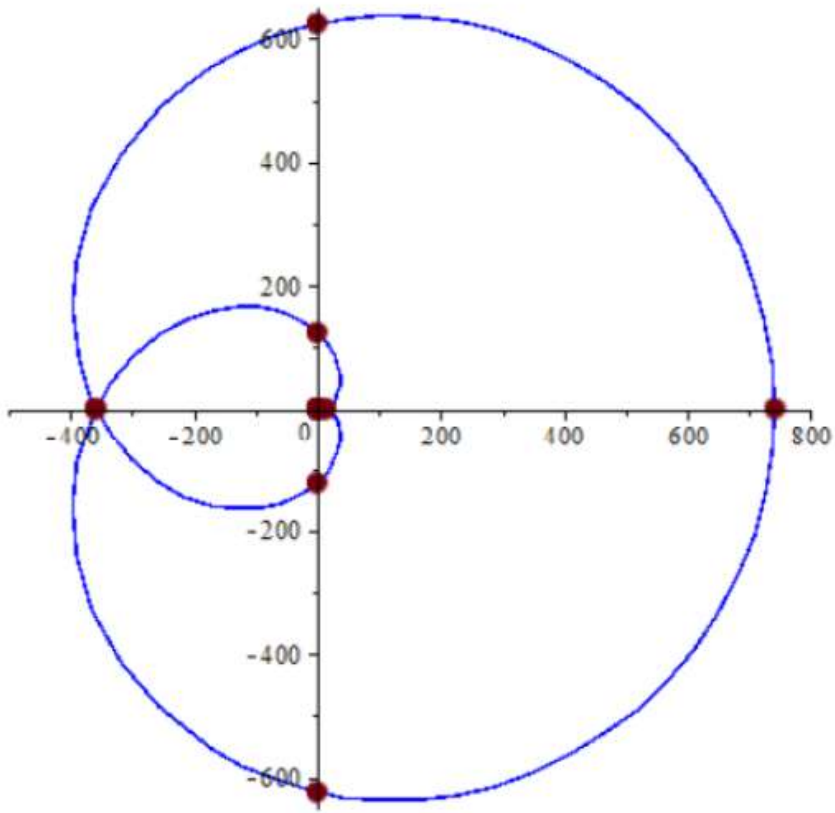


Figure 3. Lambert lines in the Z-plane

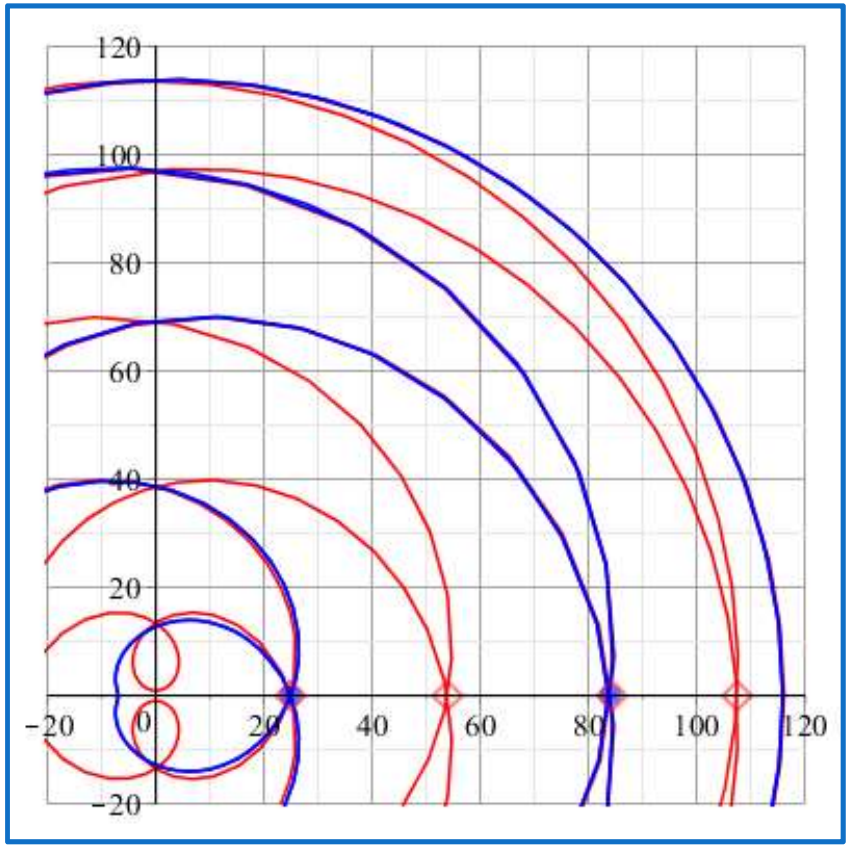
Mapping two:

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

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.



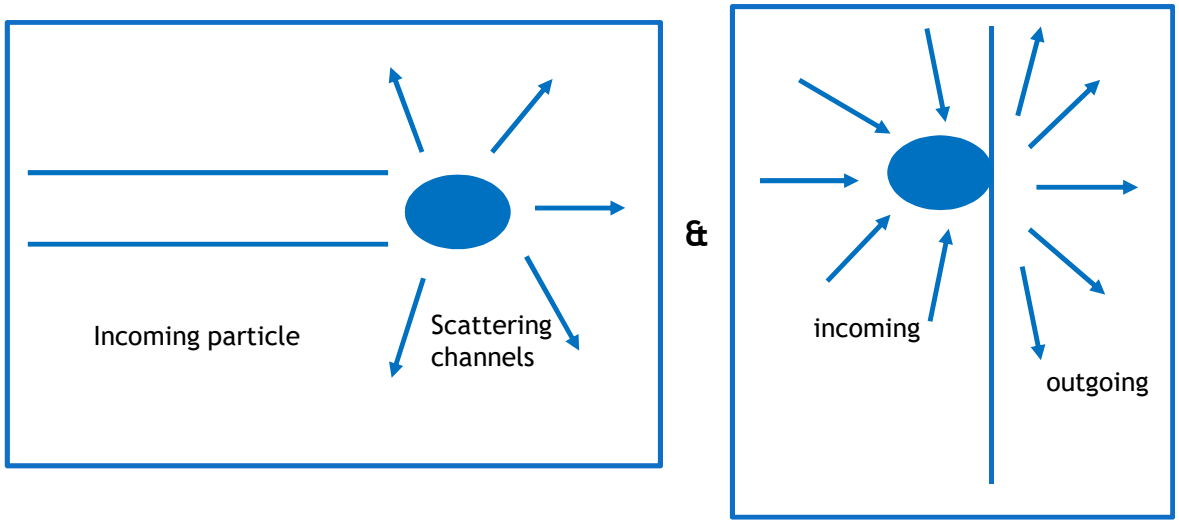
A closer view of quadrant 1 of z-plane graph. .

Looking Forward– Further Possibilities

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.