Quantum Scattering, Degrees of Freedom and Holomorphic Functions: A Comprehensive Report

Shahnaz Abdul Hameed

Submitted: 17 July 2023

Abstract

This report delves into some key topics in understanding quantum mechanical systems (and scattering): the S-Matrix and its properties, analysis of degrees of freedom for n to m transitions of stable/spinless particles, an exploration of holomorphic functions and the complex square-root function and study of Riemann Sheets. Through derivations, discussions, and visual representations, this report intends to provide a comprehensive overview of these fundamental concepts.

1 What's the S-Matrix, why do we need it

A priceless example of where studying scattering has contributed in building our understanding of the world is the **Geiger-Marsden** experiments, led by *Rutherford* between 1908 and 1913. In the experiment, a beam of α particles was scattered against a thin gold foil and the scattering angles were then measured.

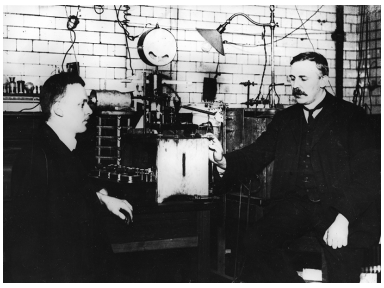


Figure 1: Rutherford and Geiger, probably talking about α ray research.

Studying the results led to a greater understanding of the atom (it was deduced that most of the atom mass is concentrated in the nucleus and has a positive charge, a pivotal result at the time!).

To further aid in scattering research, the *scattering matrix*, or **S-matrix**, was introduced by *John Archibald Wheeler* in 1937 [https://journals.aps.org/pr/abstract/10.1103/PhysRev.52.1107], later developed by *Werner Heisenberg* in the 40s The unitary property of the S-matrix is directly related to the conservation of the probability current in quantum mechanics.

In the context of QFT, the S-matrix is defined as the unitary matrix connecting sets of asymptotically free particle states (the *in-states* and the *out-states*) in the Hilbert space of physical states. This is very useful because often we cannot describe the interaction (at least, not the most interesting ones) exactly. A multi-particle state is said to be **free** (non-interacting), if it transforms under *Lorentz transformations* as a tensor product, or direct product in physics parlance, of *one-particle states*. Asymptotically free then means that the state has this appearance in either the distant past or the distant future.

While the S-matrix may be defined for any background (spacetime) that is asymptotically solvable and has no event horizons, it has a simple form in the case of *Minkowski space*. In this special case, the Hilbert space is a space of irreducible unitary representations of the inhomogeneous Lorentz group (the Poincaré group); the S-matrix is the evolution operator between $t = -\infty$ (the distant past) and $t = +\infty$ (the distant future). It is defined only in the limit of zero energy density (or infinite particle separation distance).

1.1 Mathematical formulation

For the purposes of illustration, we consider the 1-D case where S-matrix is 2-dimensional. Consider a localized one-dimensional potential barrier $V(x)$, subjected to a beam of quantum particles with energy E. These particles are incident on the potential barrier from left to right.

The solutions of *Schrödinger's equation* outside the potential barrier are plane waves given by

$$\psi_{\mathrm{L}}(x) = Ae^{ikx} + Be^{-ikx}$$

for the region to the left of the potential barrier, and

$$\psi_{\mathrm{R}}(x) = Ce^{ikx} + De^{-ikx}$$

for the region to the right of the potential barrier, where

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

is the wave vector. The term with coefficient A represents the incoming wave, while the term with coefficient C represents the outgoing wave. B stands for the reflecting wave. Since we set the incoming wave moving in the positive direction (coming from the left), D is zero and can be omitted.

The "scattering amplitude," i.e., the transition overlap of the outgoing waves with the incoming waves, is a linear relation defining the S-matrix,

$$\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix}.$$

The above relation can be written as

$$\Psi_{\text{out}} = S\Psi_{\text{in}}$$

where

$$\Psi_{\text{out}} = \begin{pmatrix} B \\ C \end{pmatrix}, \quad \Psi_{\text{in}} = \begin{pmatrix} A \\ D \end{pmatrix}, \qquad S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}.$$

The elements of S completely characterize the scattering properties of the potential barrier $V(x)$.

The probability current density J of the wave function $\psi(x)$ is defined as

$$J = \frac{\hbar}{2mi}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right).$$

1.1.1 Unitarity Property

The probability current density $J_{\text{L}}(x)$ of $\psi_{\text{L}}(x)$ to the left of the barrier is

$$J_{\text{L}}(x) = \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right),$$

while the probability current density $J_{\text{R}}(x)$ of $\psi_{\text{R}}(x)$ to the right of the barrier is

$$J_{\text{R}}(x) = \frac{\hbar k}{m}\left(|C|^2 - |D|^2\right).$$

For conservation of the probability current, $J_{\text{L}} = J_{\text{R}}$. This implies the S-matrix is a unitary matrix.
Proof

$$\begin{aligned} J_{\text{L}} &= J_{\text{R}} \\ |A|^2 - |B|^2 &= |C|^2 - |D|^2 \\ |B|^2 + |C|^2 &= |A|^2 + |D|^2 \\ \Psi_{\text{out}}^\dagger \Psi_{\text{out}} &= \Psi_{\text{in}}^\dagger \Psi_{\text{in}} \\ \Psi_{\text{in}}^\dagger S^\dagger S \Psi_{\text{in}} &= \Psi_{\text{in}}^\dagger \Psi_{\text{in}} \\ S^\dagger S &= I \end{aligned}$$

Of course, this means that the inverse of S is unitary. By definition, U is unitary if $U^\dagger U = I$. Taking the Hermitian conjugate, $(U^{-1}U)^\dagger = U^\dagger (U^{-1})^\dagger$. Since $U^\dagger U = I$, we have $(U^\dagger)^{-1} = U^{-1}$. Thus, U^{-1} is unitary.

2 n-m S matrix transition in spinless particles

In using the S-matrix to describe a scattering experiment, we will assume that the forces are of sufficiently short range that the initial and final states consist effectively of free particles. These states can then be specified by the momentum of each particle together with certain discrete quantum numbers such as the spin and isospin. Due to the finite size of any experiment, there is some residual uncertainty in the momentum, but we assume that this is unimportant in practice. The momentum eigenvalues form a continuous spectrum, but for clarity of notation in this section, we will begin by using a discrete symbol m or n to label the states.

Let $|n\rangle$ denote the initial state of two particles that subsequently come together, interact, and separate. The superposition principle in quantum mechanics tells us that the final state can be written as $S|n\rangle$, where S is a linear operator. The probability that a measurement on the final state gives a result corresponding to the state $|m\rangle$ is obtained from the square of the modulus of the matrix element:

$$\langle m|S|n\rangle$$

The set of states $|n\rangle$ is assumed to be orthonormal and complete:

$$\langle m|n\rangle = \delta_{mn}, \quad \sum_m |m\rangle\langle m| = 1.$$

We consider next the consequences of relativistic invariance. If L is any proper Lorentz transformation, and if

$$L|m\rangle = |m'\rangle,$$

we require that

$$\langle m\,|S|n\,\rangle^2 = \langle m'|S|n'\rangle^2$$

in order that observable quantities be independent of the Lorentz frame. The definition of the S-matrix elements given above does not specify the phase uniquely. This permits us to replace (1.2.7) by the stronger condition

$$\langle m\,|S|n\,\rangle = \langle m'|S|n'\rangle$$

For spinless particles, this has the consequence that the matrix elements depend on the four-momenta only through their invariant scalar products. For example, the two-particle to two-particle matrix element is given by

$$\langle p_3, p_4|S|p_1, p_2\rangle$$

Consider a system composed of n particles of mass m and m particles of mass M. Each particle has a definite 4-momentum, denoted by p_i for the i-th particle. Conservation of 4-momentum implies that the total 4-momentum of the system is conserved:

$$p_{\text{total}} = \sum p_i = 0,$$

where the sum runs over all $n + m$ particles.

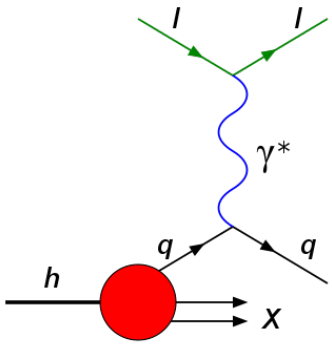
2.1 the independent kinematic variables, how free is our matrix

Consider a generic production process of the type

$$1 + 2 \ldots + n \to (n+1) + (n+2) + \ldots + m.$$

Let's analyse the number of independent Lorentz-invariant variables for this reaction.

Due to:



- the conservation of four-momentum $P_1 + P_2 \ldots P_n = P_{n+1} + P_{n+2} + \ldots + P_m$, (4 constraints);
- the mass shell conditions $p_i^2 = m_i^2$, $i = 1, 2, \ldots, m+n$ ($m+n$ constraints);
- the arbitrariness in fixing a 4-dimensional reference frame (6 constraints);

of the a priori available $4(m+n)$ variables (the components of the four-vectors P_i), only $3(m+n)-10$ remain as truly independent variables. In practice, one of these variables (e.g., the beam energy, the center-of-mass energy of the colliding particles, etc.) is fixed by preparing the initial state.

3 from Spinless particles to Holomorphic functions, a leap of faith

Before getting into the exact definition, clearing a few concepts:

- **Complex-valued function**: A mapping which assigns to each $z \in C$ a unique complex number $f(z) \in C$.
- **Complex-differentiability**: A function $f(z)$ defined on an open subset D of the complex plane is said to be *complex differentiable* at a point $z_0 \in D$ if the following limit exists:

$$f'(z_0) = \lim_{h \to 0} \frac{f(z_0 + h) - f(z_0)}{h}$$

  where h is a complex number and the limit is taken as h approaches 0.
- **Complex-coordinate space**: The complex coordinate space, denoted as C^n, represents a vector space consisting of n complex coordinates. Each coordinate can be represented as $z_i = x_i + iy_i$, where x_i and y_i are real numbers, and i is the imaginary unit. The elements of C^n can be written as vectors:

$$\mathbf{z} = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{pmatrix}$$

where $\mathbf{z}$ is a column vector in C^n.

3.1 getting into holomorphism

A function $f(z)$ defined on a complex domain is said to be **holomorphic** if it is *complex differentiable* at every point within that domain. In other words, the derivative $f'(z)$ exists at each point z within the domain.

Holomorphism brings in several convenient properties. For example, they are analytic, meaning they can be locally represented by a convergent power series expansion. Additionally, the *Cauchy-Riemann* equations provide a necessary and sufficient condition for a function to be holomorphic.

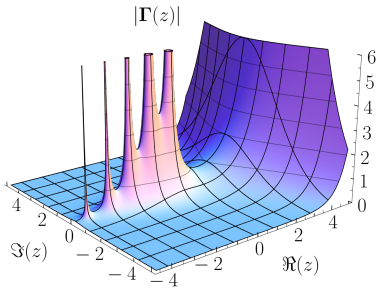
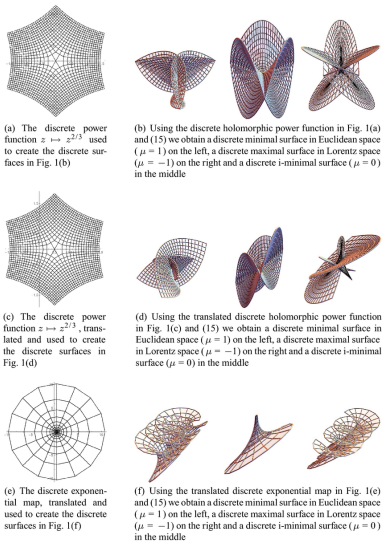


Figure 2: a 3-d plot of absolute value of complex γ function

Examples of holomorphic functions:

- Polynomial functions: $f(z) = a_n z^n + a_{n-1} z^{n-1} + \ldots + a_1 z + a_0$, where $a_n, a_{n-1}, \ldots, a_1, a_0$ are complex constants.
- Exponential function: $f(z) = e^z$, where e is the base of the natural logarithm.
- Trigonometric functions: $f(z) = \sin(z)$, $f(z) = \cos(z)$, $f(z) = \tan(z)$, etc.
- Rational functions: $f(z) = \frac{P(z)}{Q(z)}$, where $P(z)$ and $Q(z)$ are polynomials.



(a) The discrete power function $z \mapsto z^{2/3}$ used to create the discrete surfaces in Fig. 1(b)

(b) Using the discrete holomorphic power function in Fig. 1(a) and (15) we obtain a discrete minimal surface in Euclidean space ($\mu = 1$) on the left, a discrete maximal surface in Lorentz space ($\mu = -1$) on the right and a discrete i-minimal surface ($\mu = 0$) in the middle

(c) The discrete power function $z \mapsto z^{2/3}$, translated and used to create the discrete surfaces in Fig. 1(d)

(d) Using the translated discrete holomorphic power function in Fig. 1(c) and (15) we obtain a discrete minimal surface in Euclidean space ($\mu = 1$) on the left, a discrete maximal surface in Lorentz space ($\mu = -1$) on the right and a discrete i-minimal surface ($\mu = 0$) in the middle

(e) The discrete exponential map, translated and used to create the discrete surfaces in Fig. 1(f)

(f) Using the translated discrete exponential map in Fig. 1(e) and (15) we obtain a discrete minimal surface in Euclidean space ($\mu = 1$) on the left, a discrete maximal surface in Lorentz space ($\mu = -1$) on the right and a discrete i-minimal surface ($\mu = 0$) in the middle

4 Complex Roots

We can unambiguously define the square root of a positive real number. But when it gets to complex numbers, representations get a little tricky. We can ease into it starting from some fundamental concepts.

4.1 Euler's formula

We can associate a complex number with the point in the plane that has Cartesian coordinates (x, y).

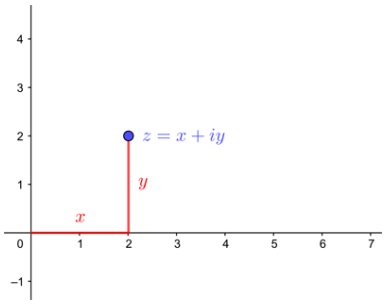


Figure 3: A complex number represented as a point on the plane in Cartesian coordinates

Euler's formula tells us that z can also be written as

$$z = re^{i\theta},$$

where (r, θ) are the polar coordinates of the point in the plane associated to z. Here r is the distance from that point to the point $(0, 0)$, and θ is the angle formed by the line connecting the point to $(0, 0)$ and the positive x-axis (measured anticlockwise).

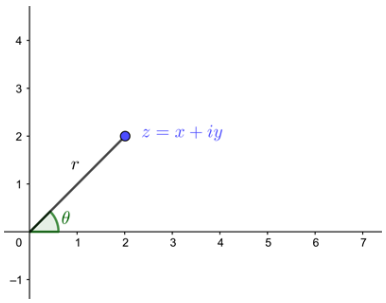


Figure 4: A complex number represented as a point on the plane in polar coordinates

4.2 taking the square root

When it comes to the square root of a complex number $z = re^{i\theta}$ we again have two options, as we did for square roots of real numbers. The first is

$$\sqrt{r}e^{i\frac{\theta}{2}}.$$

Let's just check this works:

$$\left(\sqrt{r}e^{i\frac{\theta}{2}}\right)^2 = \sqrt{r}^2\left(e^{i\frac{\theta}{2}}\right)^2 = re^{i\theta},$$

as required.

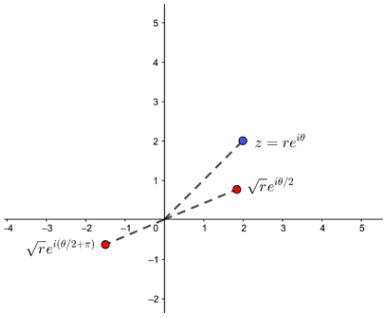
The second option is

$$\sqrt{r}e^{i(\frac{\theta}{2}+\pi)}.$$

Again let's check:

$$\left(\sqrt{r}e^{i(\frac{\theta}{2}+\pi)}\right)^2 = \sqrt{r}^2\left(e^{i(\frac{\theta}{2}+\pi)}\right)^2 = re^{i(\theta+2\pi)} = re^{i\theta},$$

as required.



Our two expressions,

$$\sqrt{r}e^{i\frac{\theta}{2}} \quad \text{and} \quad \sqrt{r}e^{i(\frac{\theta}{2}+\pi)}$$

are called the two *branches* of the square root.

4.3 making a function, multivaluedness

Consider what happens as you approach a point on the negative real line from above and from below. We can approach the point from above by looking at points $z = re^{i\theta}$ with θ increasing from 0 to π. Since our function is

$$f(z) = \sqrt{r}e^{i\frac{\theta}{2}},$$

the value of $f(z)$ approaches

$$\sqrt{r}e^{i\frac{\pi}{2}} = \sqrt{r}i.$$

To approach our point from below we can look at points $z = re^{i\theta}$ with θ decreasing from 0 to $-\pi$. Since our function is

$$f(z) = \sqrt{r}e^{i\frac{\theta}{2}},$$

the value of $f(z)$ now approaches

$$\sqrt{r}e^{-i\frac{\pi}{2}} = -\sqrt{r}i.$$

Therefore, if we defined our function as

$$f(z) = \sqrt{r}e^{i\frac{\theta}{2}}$$

on the whole complex plane, it would not be continuous on the negative real line. As we approach a point z on the negative real line from above, the function $f(z)$ approaches $\sqrt{r}i$, but as we approach z from below, the function approaches $-\sqrt{r}i$.

The problem of the discontinuity doesn't occur just because we chose the "wrong" branch to define our function. If we had chosen to define the function as

$$f(z) = \sqrt{r}e^{i(\frac{\theta}{2}+\pi)}$$

in an analogous way, it would also have been discontinuous on the negative real line.

In summary, the complex square root is a *multi-valued* function that can't be defined unambiguously on the whole complex plane in a way that makes it continuous.

4.4 the consequent need for a new surface, a more fitting representation

We start by taking two copies of the complex plane and cutting each along the negative real axis (such a cut is called a branch cut). On one copy of this cut complex plane we define

$$f(z) = \sqrt{r}e^{i\frac{\theta}{2}},$$

and on the other we define

$$f(z) = \sqrt{r}e^{i(\frac{\theta}{2}+\pi)}.$$

Now we glue the top edge of the cut of the first copy to the bottom edge of the cut of the second copy, and vice versa. On the resulting surface (called a Riemann surface) the square root function is now defined unambiguously and continuously.

To illustrate this, look at points $z = re^{i\theta}$ on the first copy, with $0 < \theta < \pi$. As you increase θ towards π, so you approach the top edge of the cut in the first copy of the plane, the function

$$f(z) = \sqrt{r}e^{i\frac{\theta}{2}}$$

approaches $\sqrt{r}i$.

Now look at points $z = re^{i\theta}$ on the second copy, with $0 > \theta > -\pi$, and decrease θ towards $-\pi$. This means you are approaching the bottom edge of the cut on the second copy of the plane. Since on that second copy the function is defines as

$$f(z) = \sqrt{r}e^{i(\frac{\theta}{2}+\pi)},$$

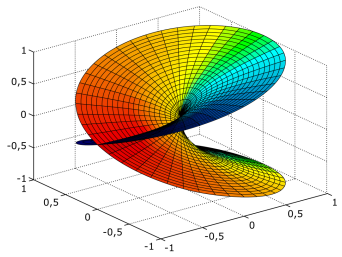
the value of $f(z)$ approaches

$$f(z) = \sqrt{r}e^{i(-\frac{\pi}{2}+\pi)} = \sqrt{r}e^{i\frac{\pi}{2}} = \sqrt{r}i$$

as θ approaches $-\pi$.

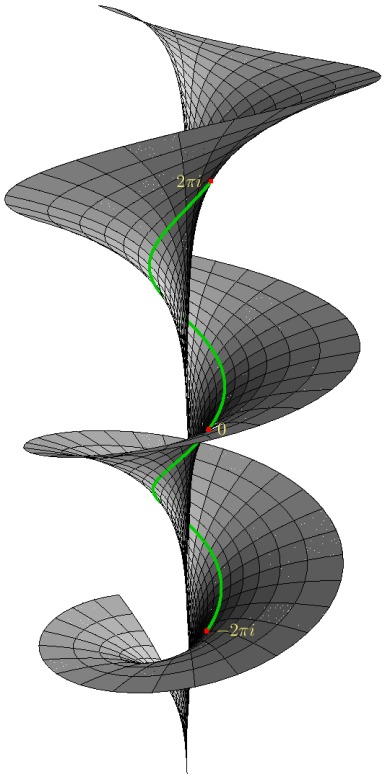
And since the top edge of the cut in the first copy of the plane has been glued to the bottom edge of the cut in the second copy of the plane, the function is now continuous on the line that comes from gluing together the two edges.

This is an illustration of the Riemann surface that comes from the cutting and gluing:



Once you have glued the top edge of the cut of one copy of the plane to the bottom edge of the cut of the other copy of the plane, the two remaining free edges of the cut end up on different sides of the surface you have created so far. So the only way to glue those free edges together is to **allow the surface to pass through itself**. This is why a three-dimensional representation of this Riemann surface intersects itself.

Another example is the complex logarithm, which actually has infinitely many values. In this case the associated Riemann surface is a beautiful infinite stair case (of which a finite section is shown below).

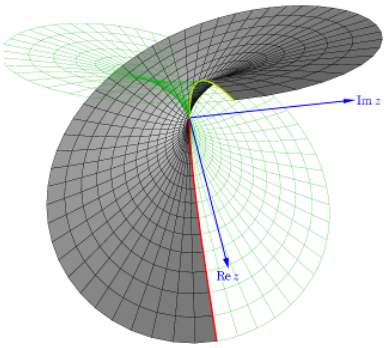


$z = \operatorname{Re}\log(x+iy) + \operatorname{Im}\log(x+iy)$

4.4.1 cutting and gluing?

Look at the Riemann surface of $f(z) = \sqrt{z}$, so the set $\{(z, w) \in C^2 : w^2 = z\}$. The point of the Riemann surface is to understand this multi-valued function. To *see* z and w, we need an embedding, not just the abstract description by "gluing slit planes".

Below is the Riemann surface of $w = \sqrt{z}$, orthogonally projected into the 3-dimensional space containing the z (complex) line and the real axis of w. The blue axes span the z line. The two points above/below a z-value have as their vertical coordinate the real parts of the two square roots of z.



The shaded branch and the transparent branch are each defined on the complement of the non-negative reals. Each "interpolates" between the positive (yellow) and negative (red) real square root. (It's not easy to "see" the w-values here, since the imaginary part of w has been projected out.)

4.5 playing around with Riemann Sheets

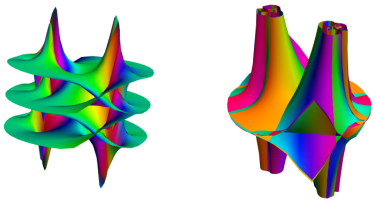
The Mathematica code below (by https://mathematica.stackexchange.com/users/9490/jason-b) defines a function rsurf that generates a grid with two Riemann surface plots of a given complex function, showcasing the real and imaginary parts with specific colorings based on their values.

```
rsurf[func_] := Grid[{{
RiemannSurfacePlot3D[w == func, Re[w],
{z, w},
ImageSize -> 400,
Coloring -> Hue[Rescale[ArcTan[1.4 Im[w]],
{-Pi/2, Pi/2}]],
PlotPoints -> {40, 40}, Boxed -> False],
RiemannSurfacePlot3D[w == func, Im[w],
{z, w},
ImageSize -> 400,
Coloring -> Hue[Rescale[ArcTan[1.4 Re[w]],
{-Pi/2, Pi/2}]],
PlotPoints -> {40, 40}, Boxed -> False]}};
```

Let's analyse some convoluted, interesting and beautiful riemann sheets simulated from complicated functions.

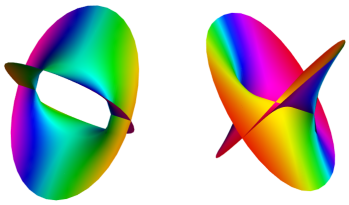
- $$w(z) = \tanh(k\sqrt{1 - z^2}) - \frac{2iz\sqrt{1 - z^2}}{1 - 2z^2}$$

```
With[{k = 1 + 2 I},
 rsurf[Tanh[k Sqrt[1 - z^2]]
 - 2 I z Sqrt[1 - z^2]/(1 - 2 z^2)]
 ]
```



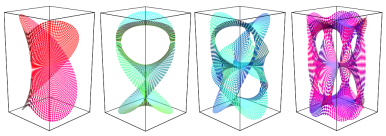
- $$w(z) = \sqrt{1 - z^2}$$

```
rsurf[Sqrt[1 - z^2]]
```



Lastly, Riemann surfaces for solutions of the equation

$[w(z)]^d + w(z) + z^{d-1} = 0.$; for d=2, 3, 4 and 5.



5 Summary

The report begins by practical definitions of the **S-matrix** (or the *scattering matrix*, in other parlance) as well it's mathematical treatment. It derives an expression for the **degrees of freedom** from n to m state transition of spinless particles (from energy-mass formula and conservation laws). It then goes on to analyse **holomorphic functions**, the concepts at its base and square root function of complex arguments. A mathematical pivot is set up for understanding and treating **complex square root functions**, by using branch-cuts and *Riemann sheets* to represent *multivaluedness*. Similar functions are explored and simulated on Mathematica. I sincerely thank Prof. Maxim Mai for his thorough theoretical guidance of the S-Matrix theory and its peripherals.