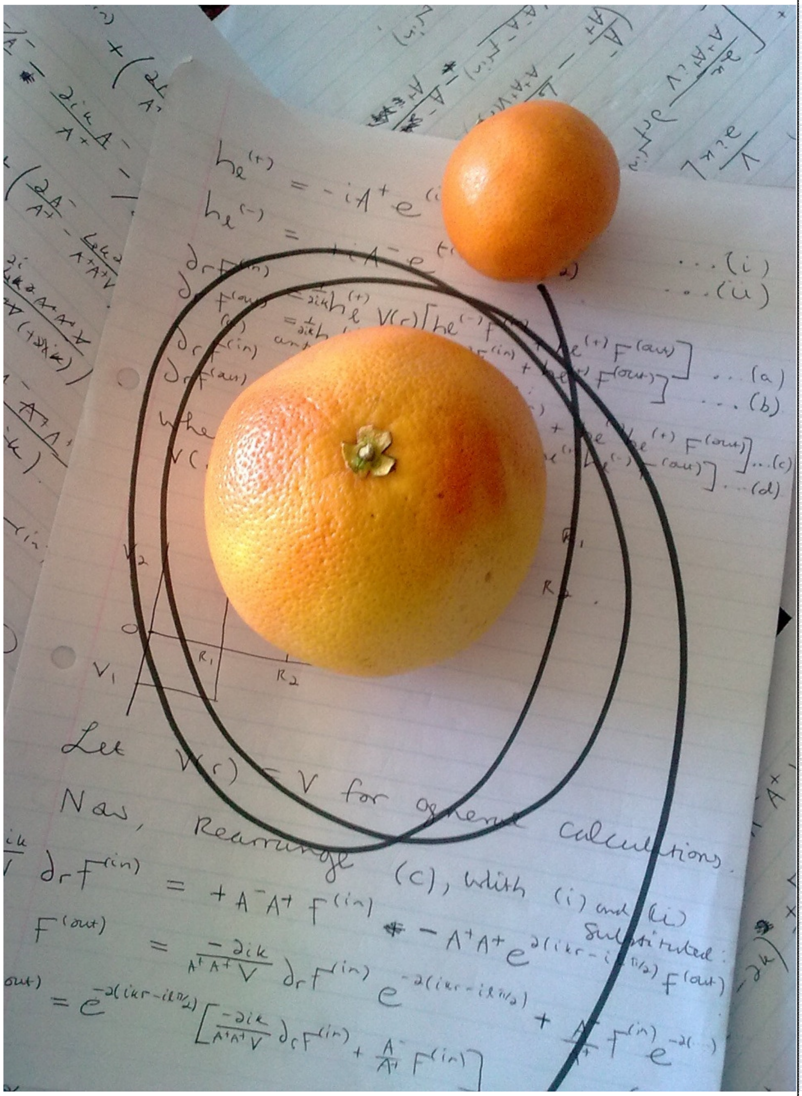
A Study of Resonant- and Bound-State Dependence on the Variables of a Step-Potential for a Quantum Mechanical System by making use of Jost Functions



An Honours Degree
Project
in Physics
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1. Abstract

System stability is a fundamental concept in understanding nature. In other words, one must be able to determine if a system of particles in a specific scenario can exist indefinitely, or if some sort of decay will take place. This can provide information on, among others, nuclear and chemical reactions, nuclear decay, and specifically particle scattering.

In this paper, resonant and bound state energies for a system of particles with a given step-potential are calculated by making use of the Jost equations for the system. By varying the equivalent mass, radii and potential magnitudes, the energy of the system is affected, thus the state of the system is also affected: this relationship between the potential variables and the state of the system is thoroughly researched for the specific potential.

It is discovered that an increase in the equivalent mass of the system results in a proportional increase in bound states and in bound state energies, as well as a decrease in resonant state energies and resonance state widths.

Potential depth and sharpness also affect the number of bound states, where greater values of an attractive potential results in a proportional increase in bound states and a decrease in virtual states. Greater values of a repulsive potential result in fewer bound states.

Where the attractive and repulsive potentials have the same values, there is an increase in bound state energies for large values, yet there is no increase in the number of bound states. Virtual states exist for small values, but these disappear for larger, wider potential peaks. Resonances are of smaller energies and width for systems of smaller, narrower potential peaks.

2. Introduction

No system with an easily defined step-potential, as we are using, occurs in nature. Yet it may be used as a reasonably accurate approximation for certain scenarios. It simplifies calculations, and enables us to solve most of the equations pertaining to the problem analytically.

The system will be considered non-relativistically, since most systems involving particles at the quantum level belong to this category.

In this introduction, I will begin by giving a brief overview of the basic principles of Quantum Mechanics, specifically introducing Schrödinger's Equation, from which the Jost equations are derived. The possible states in which a system can exist are then discussed. The relationship between these states and the Jost equations are of specific importance, and it is explained in detail.

2.1 The Basics of Quantum Mechanics & Deriving the Time-Independent Schrödinger's Equation

At a specific time, a system will be in a state that can be described by a full set of conserving quantum numbers, like total energy, angular momentum and spin. We will denote this set as:

$$a = \{\alpha_1, \alpha_2, \dots, \alpha_N\} \tag{1}$$

In co-ordinate notation, the state can be fully described by the complex-valued wave function, $\Psi_\mathrm{a}(\mathrm{t}, \mathbf{r})$. It is dependent on time, the spatial orientation, as well as the set of quantum numbers pertaining to the system. The density of states, or the probability of finding a particle in a specific configuration at any instant of time, is the squared absolute value of the wave function.

To gain any information about a system, like finding the bound and resonant states, it appears that the wave function for the system must be calculated. For no better reason than "it just works", we turn to Schrödinger's equation to do just that:

$$i\hbar \frac{\partial}{\partial t} \Psi_a(t, \boldsymbol{r}) = \boldsymbol{H}\, \Psi_a(t, \boldsymbol{r}) \tag{2}$$

$\boldsymbol{H}$ denotes the Hamiltonian operator. It is comprised of the kinetic energy operator (the free motion Hamiltonian) and the potential energy operator (sum of inter-particle potentials and a potential generated by an external field). The Hamiltonian can thus be understood as the total energy operator. The symbol ħ of course denotes Planck's constant.

Schrödinger's equation determines the state of the system at any time, t, if it is known at a specific time $t = t_0$. We will apply the method of separation of variables to (2), Schrödinger's equation, to attempt to get rid of the time dependence. Therefore we let:

$$\Psi_a(t, \boldsymbol{r}) = X(t)\psi_a(\boldsymbol{r}) \tag{3}$$

Where $X(t)$ is a time dependant function, and $\psi_a(\boldsymbol{r})$ is spatially dependant, as well as being dependant on the quantum numbers, denoted by the subscript a. We then take the time derivative of (3) and multiply it by a factor $i\hbar$:

$$\therefore\ i\hbar \frac{\partial}{\partial t} \Psi_a(t, \boldsymbol{r}) = i\hbar \frac{\partial X(t)}{\partial t} \psi_a(\boldsymbol{r}) \tag{4}$$

We now substitute (2) into (4):

$$\therefore\ \boldsymbol{H}\, \Psi_\mathrm{a}(t, \boldsymbol{r}) = i\hbar \frac{\partial X(t)}{\partial t} \psi_a(\boldsymbol{r})$$

We also substitute (3) into this expression:

$$\therefore\ \boldsymbol{H}\, [X(t)\psi_a(\boldsymbol{r})] = i\hbar \frac{\partial X(t)}{\partial t} \psi_a(\boldsymbol{r}) \tag{5}$$

We assume that the Hamiltonian operator is time-independent, and that it will thus be conserving. This assumption may seem rash, but it hinges on the fact that energy cannot be created or destroyed from nothing, and that the total energy of a finite system must thus remain constant. No contradictory occurrence has been empirically observed. Our assumption is thus justified. Thus:

$$\boldsymbol{H}\,[X(t)\psi_a(\boldsymbol{r})] = X(t)\,\boldsymbol{H}\,\psi_a(\boldsymbol{r}) = X(t)E\,\psi_a(\boldsymbol{r}) = E\,X(t)\psi_a(\boldsymbol{r})$$

Where E is the energy eigenvalue corresponding to the $\boldsymbol{H}$ operator. E can be chosen as one of the quantum numbers of the system, since $\boldsymbol{H}$ is conserving. So we then have:

$$\boldsymbol{H}\,\psi_a(\boldsymbol{r}) = E\,\psi_a(\boldsymbol{r}) \tag{6}$$

This is the time-independent Schrödinger's equation, which is of great importance later. Returning to the differential equation (5), with (6) taken into account:

$$\mathrm{E}\,X(t)\psi_a(\boldsymbol{r}) \;=\; i\hbar\frac{\partial X(t)}{\partial t}\psi_a(\boldsymbol{r})$$

$$\therefore\;\mathrm{E}\,X(t) \;=\; i\hbar\frac{\partial X(t)}{\partial t}$$

Solving this differential equation yields:

$$X(t) \;=\; exp\,(-\frac{i}{\hbar}Et) \tag{7}$$

This is the time dependant part of Schrödinger's equation. When substituting (7) into (3), the solution to Schrödinger's equation becomes:

$$\Psi_a(t,\boldsymbol{r}) = exp\left(-\frac{i}{\hbar}Et\right)\psi_a(\boldsymbol{r}) \tag{8}$$

Note that the application of the method of separation of variables would be pointless if the Hamiltonian was not conserving. Thus this is a fundamental prerequisite for most problems in Quantum Mechanics.

All that remains is to calculate the time-independent wave equation by means of equation (6), the time-independent Schrödinger's equation. In future, where the wave equation and Schrödinger's equation is mentioned, assume that the time-independent wave equation and the time-independent Schrödinger's equation is referred to, unless otherwise stated.

2.2 Schrödinger's Equation in Spherical Co-ordinates

We will be dealing with a radial potential in this scenario, thus it would be wise to attempt to convert the time-independent Schrödinger's equation to a more fitting set of co-ordinates. Consider the Hamiltonian, $\boldsymbol{H}$, comprised of Kinetic Energy Operator and Potential Energy:

$$\boldsymbol{H} = \frac{\boldsymbol{p}^2}{2\mu} + U(\boldsymbol{r})$$

Where $\boldsymbol{p}$ denotes the momentum operator, μ the equivalent mass of the particles under consideration, and $U(\boldsymbol{r})$ the potential. From the definition of $\boldsymbol{p}$, the Hamiltonian can be written as:

$$\boldsymbol{H} = -\frac{\hbar^2}{2\mu}\boldsymbol{\Delta} + U(\boldsymbol{r}) \tag{9}$$

With $\boldsymbol{\Delta}$ denoting the Laplacian, given, in spherical co-ordinates in terms of the angular momentum operator, by:

$$\boldsymbol{\Delta} = \frac{1}{r^2}\partial_r(r^2\partial_r) - \frac{1}{\hbar^2 r^2}\boldsymbol{L}^2 \tag{10}$$

$\boldsymbol{L}$ denotes the angular momentum operator (which, by the way, is conserving). Substituting (10) into (9) yields:

$$\boldsymbol{H} = -\frac{\hbar^2}{2\mu}\frac{1}{r^2}\partial_r(r^2\partial_r) + \frac{1}{2\mu r^2}\boldsymbol{L}^2 + U(\boldsymbol{r}) \tag{11}$$

When substituting (11) into (6), Schrödinger's Equation becomes:

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\partial_r(r^2\partial_r) + \frac{1}{2\mu r^2}\boldsymbol{L}^2 + U(\boldsymbol{r})\right]\psi_a(\boldsymbol{r}) = E\,\psi_a(\boldsymbol{r}) \tag{12}$$

Notice that the potential function is also dependant on the spatial vector. We consider a radial step-potential, thus U is only dependant on r, the radial distance from a point of reference. We now make the following substitutions:

$$k^2 = \frac{2\mu E}{\hbar^2} \tag{13}$$

$$V(r) = \frac{2\mu}{\hbar^2}U(r) \tag{14}$$

k is called the momentum of the propagating spherical wave. The reason for these substitutions will soon become clear.

Again using the technique of separation of variables, we can write $\psi_a(\boldsymbol{r})$ as a product of a radially dependant function and an angular dependant function. This is a simple task, since the well-studied spherical harmonics, denoted by $Y_{lm}(\theta,\varphi)$, form a complete basis in the subspace of the spherical angles. Thus we can write:

$$\psi_a(\boldsymbol{r}) = \frac{u_l(r)}{r}\,Y_{lm}(\theta,\varphi) \tag{15}$$

The factor $\frac{1}{r}$ is introduced to simplify (12), but it is not necessarily of cardinal importance. The sperical harmonics have, among others, the following property:

$$\boldsymbol{L}^2 Y_{lm}(\theta,\varphi) = l(l+1)\,\hbar^2 Y_{lm}(\theta,\varphi) \tag{16}$$

Where l is the conserving angular momentum eigenvalue, since $\boldsymbol{L}$ is conserving. The significance and meaning of the other conserving quantum number, m, is not discussed here: it is not required in our calculations.

It should be clear why the spherical harmonics are introduced now: substituting (16) into (12) will effectively get rid of the $\boldsymbol{L}^2$ operator. Indeed, $Y_{lm}(\theta,\varphi)$ is the eigenfunction of $\boldsymbol{L}$. Thus it will not act on $u_l(r)$; the subscript l indicates that the function is dependent on l, though, but this is only through $Y_{lm}(\theta,\varphi)$.

One last remark before attacking (12): The subscript a is tediously included when writing $\psi_a(\boldsymbol{r})$. This is to indicate the wave equation's dependence on quantum numbers as yet unknown, although energy is identified as a quantum number early in the calculations. It should be clear from (15) though, that the set of quantum numbers sufficient to determine $\psi_a(\boldsymbol{r})$, for our purposes, at least, is given by:

$$a = \{E, l, m\} \tag{17}$$

Now let us substitute (13) – (15) into (12) and apply (16):

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\partial_r\left(r^2\partial_r\left(\frac{u_l(r)}{r}\,Y_{lm}(\theta,\varphi)\right)\right)+\frac{1}{2\mu r^2}\boldsymbol{L}^2\frac{u_l(r)}{r}\,Y_{lm}(\theta,\varphi)+U(r)\frac{u_l(r)}{r}\,Y_{lm}(\theta,\varphi)$$

$$= E\,\frac{u_l(r)}{r}\,Y_{lm}(\theta,\varphi)$$

$$\therefore -\frac{1}{r^2}\partial_r\left(r^2\partial_r\left(\frac{u_l(r)}{r}\right)\right)Y_{lm}(\theta,\varphi)+\frac{2\mu}{\hbar^2}\frac{1}{2\mu r^2}\frac{u_l(r)}{r}l(l+1)\,\hbar^2\,Y_{lm}(\theta,\varphi)$$

$$+\frac{2\mu}{\hbar^2}U(r)\frac{u_l(r)}{r}\,Y_{lm}(\theta,\varphi)=\frac{2\mu}{\hbar^2}E\,\frac{u_l(r)}{r}\,Y_{lm}(\theta,\varphi)$$

Note that the spherical harmonics cancel:

$$\therefore -\frac{1}{r^2}\partial_r\left(r^2\left(\frac{r\partial_r u_l(r)-u_l(r)}{r^2}\right)\right)+\frac{1}{r^2}\frac{u_l(r)}{r}l(l+1)+V(r)\frac{u_l(r)}{r}\ =k^2\ \frac{u_l(r)}{r}$$

$$\therefore -\frac{1}{r^2}\partial_r\big(r\partial_r u_l(r)-u_l(r)\big)+\frac{1}{r^2}\frac{u_l(r)}{r}l(l+1)+V(r)\frac{u_l(r)}{r}\ =k^2\ \frac{u_l(r)}{r}$$

$$\therefore -\big(r\partial_r^2 u_l(r)+\partial_r u_l(r)-\partial_r u_l(r)\big)+\frac{u_l(r)}{r}l(l+1)+rV(r)u_l(r)\ =rk^2u_l(r)$$

$$\therefore -\partial_r^2 u_l(r)+\frac{u_l(r)}{r^2}l(l+1)+V(r)u_l(r)\ =k^2u_l(r)$$

$$\therefore \partial_r^2 u_l(r)+k^2u_l(r)-\frac{l(l+1)}{r^2}u_l(r)-V(r)u_l(r)\ =0$$

Thus we finally have:

$$\left[\partial_r^2 + k^2 - \frac{l(l+1)}{r^2} - V(r)\right] u_l(r) \; = 0 \tag{18}$$

This is the radial time-independent Schrödinger's equation.

2.3 The Jost Functions

As per usual with any differential equation, boundary conditions need to be imposed to find the final solution. We apply these boundary conditions at the ends of the interval, $r \in [0, \infty)$; thus at $r = 0$ and $r \to \infty$. Since $\psi_a(\boldsymbol{r})$ must be finite everywhere, it is clear from (15) that $u_l(0) = 0$ to prevent $\psi_a(\boldsymbol{r})$ from blowing up to infinity.

At large values of r, we will assume that $V(r)$ tends to zero. To be precise, $V(r)$ need only diminish faster than $\frac{1}{r^2}$, the electrostatic potential, when $r \to \infty$ for (18) to become the "free" radial Schrödinger's equation:

$$\left[\partial_r^2 + k^2 - \frac{l(l+1)}{r^2}\right] u_l(r) = 0; \qquad r \to \infty \tag{19}$$

The solutions to (19) are either the linearly-independent Riccati-Bessel and Riccati-Neumann functions, or the pair of linearly-independent Riccati-Hankel functions. We will refrain from going into the detail of these functions, since much information is available in any Calculus textbook. It is sufficient to accept that they are solutions to the problem at hand.

All these functions behave exponentially. Also, the former can be written in terms of the latter, and vice-versa. We choose to work with the Riccati-Hankel functions, since one of the pair represents an incoming spherical wave, and the other an outgoing spherical wave. With the Riccati-Bessel and Riccati-Neumann functions, there is no such distinction.

The Riccati-Hankel functions are denoted by $h_l^{(\pm)}(kr)$, with the $-$ denoting an incoming and + denoting an outgoing spherical wave. $u_l(r)$ is a linear combination of these two functions:

$$u_l(r) = C_1 h_l^{(-)}(kr) + \; C_2 \, h_l^{(+)}(kr); \quad r \to \infty$$

With C_1 and C_2 constants that are dependant on the total energy. The energy determines wether the system is in the bound or resonant state. Thus these constants are related to the state of the system. They are, in fact, the Jost functions. Since they are functions of the total energy, we can write them as follows:

$$C_1 = f_l^{(in)}(E)$$

$$C_2 = f_l^{(out)}(E)$$

This somewhat unorthodox notation simplifies matters considerably: Both depend on the total energy, and are thus written as functions of total energy. Also, the subscript l indicates the dependence on the angular momentum. Most importantly, the "in" indicates the correspondence of the constant to the incoming spherical wave, and the "out" the correspondence of the constant to the outgoing spherical wave. The solution is then written as:

$$u_l(r) = f_l^{(in)}(E)h_l^{(-)}(kr) + f_l^{(out)}(E)h_l^{(+)}(kr); \quad r \to \infty \tag{20}$$

With the Riccati-Hankel functions given as:

$$h_l^{(\pm)}(kr) = \mp i\, e^{\pm i(kr - \frac{l\pi}{2})}; \quad r \to \infty \tag{21}$$

Thus we have:

$$u_l(r) = f_l^{(in)}(E)\, i\, e^{-i(kr-\frac{l\pi}{2})} - f_l^{(out)}(E)\, i\, e^{+i(kr-\frac{l\pi}{2})}; \quad r \to \infty \tag{22}$$

Note that this is only valid if $r \to \infty$. Otherwise, the Riccati-Hankel functions cannot be written analytically if a value for l is not specified.

We now know what the Jost functions *are*, and we know why they are significant since they are related to the state of the system: if it is bound or resonant. We will consider each case separately to glean more information from this relationship.

2.3.1 Bound States

We understand a bound state as a state in which the particles in the system are "fixed"; they cannot escape, or rather, they are bound together (hence the name). A typical Classical example is that of planetary orbit: due to the specific energy of the system, the Moon will remain in orbit of the Earth. Note that movement is still a possibility. Things are very much the same in the quantum scale: Particles cannot escape a system if the energy of the system does not allow it. The system is then in the Bound state.

Thus, in a bound state, the particle cannot leave the source of the attractive field. The probability of finding the particle when $r \to \infty$ thus tends to zero. This implies that the wave function must also tend to zero, which in turn implies that:

$$\psi_a(\boldsymbol{r}) \to 0 \quad when \quad r \to \infty \tag{23}$$

From (15) it is thus clear that:

$$u_l(r) \to 0 \quad when \quad r \to \infty \tag{24}$$

Since the total probability of finding the particle somewhere around the source of the potential is 1, the fact that $u_l(r)$ steadily disappears as $r \to \infty$ means that $\psi_a(\boldsymbol{r})$ must be square-integrable. This is the case if $f_l^{(in)}(E)$ is zero.

Also, since the potential vanishes at large r values, the implication is that the energy must be negative. If this is the case, k must be imaginary, as is clear from (13):

$$k^2 = \frac{2\mu E}{\hbar^2}$$

$$\therefore k^2 = \frac{-2\mu|E|}{\hbar^2}$$

$$\therefore k = i\sqrt{\frac{2\mu|E|}{\hbar^2}}$$

$$\therefore k = i\kappa; \quad \kappa > 0$$

When substituting this expression in (22):

$$u_l(r) = f_l^{(in)}(E)\, i\, e^{-i(i\kappa r - \frac{l\pi}{2})} - f_l^{(out)}(E)\, i\, e^{+i(i\kappa r - \frac{l\pi}{2})}; \quad r \to \infty$$

$$\therefore u_l(r) = f_l^{(in)}(E)\, i\, e^{(+\kappa r + \frac{l\pi i}{2})} - f_l^{(out)}(E)\, i\, e^{(-\kappa r - \frac{l\pi i}{2})}; \quad r \to \infty$$

The second term will thus tend to zero, and the first will tend towards infinity. For (24) to remain true, $f_l^{(in)}(E)$ must be zero, which reaffirms what was established earlier.

The real values for E such that $f_l^{(in)}(E) = 0$ will thus be the values of the total energy such that the system is in the bound state. It should be clear that the above is only applicable for real values of E, since k would otherwise not necessarily be strictly imaginary. Hence the condition: E must be real and negative.

The “old-fashioned” way, shall we say, of determining the bound state energies of a system would be to calculate the wave equation, a most tedious venture, and then to find the values of E such that it becomes zero as $r \to \infty$. In our method, we simply need to calculate the Jost functions.

2.3.2 Resonant States

Resonance is a phenomenon that presents itself in most branches of physics. Once again, a classical example is worthy of consideration:

When an asteroid approaches a planet, depending on its kinetic energy, trajectory, and the gravitational force between it and the planet, it might collide with the planet and stick to it, or orbit the planet, which would correspond to a bound state. It might also complete a number of revolutions around the planet before moving away, or collide and move away – a classical equivalent of a resonant state. The more revolutions, the longer the resonance “lives”, as it were. It is similar to the bound state, since the resonance will “live” indefinitely in such a state.

The quantum scenario is very much the same, apart from the obvious fact that Newtonian Physics cannot apply. For quantum resonances, particles will form a partially localised state, which slowly decays. This is why the terms quasi-bound, and quasi-stationary state, are sometimes used to describe them.

The problem with quantum resonances is that it cannot be defined as rigorously as bound states, although there is much similarity between the two states. Our definition hinges on the fact that resonances do not “remember” how they are formed, implying that there is no preferred direction for decay. Unrest should occur when terms such as “remember” is used for a particle, thus an example is given to better illustrate what is meant:

The oxygen isotope ${}^{16}_{8}O^{*}$ in the exited state can be formed in a number of ways: A photon might have been absorbed by ${}^{16}_{8}O$, or the isotope ${}^{15}_{8}O$ might have captured a neutron. In fact, there are a number of possible nuclear reactions. We can consider ${}^{16}_{8}O^{*}$ as a resonant state of oxygen, due to its temporary existence; It must decay at some stage due to instability. If we consider a sample of ${}^{16}_{8}O^{*}$, in other words considering an ensemble of such resonant states, the decay is random and in all directions, i.e. the decay occurs isotropically.

We can thus conclude that only the outgoing spherical wave part will be included in (22) as $r \to \infty$ and that $f_l^{(in)}(E) = 0$ for this to occur. This condition is identical to that of a bound state, hence the similarity between the two states. There is more that can be said about resonances, though:

The decay of an ensemble of resonance states can be modelled by the radioactive decay law:

$$N(t) = N_0 e^{-\frac{\Gamma}{\hbar}t} \tag{25}$$

Where $N(t)$ is the number of states at time t, N_0 is the number of states initially, and Γ is known as the resonance width, measured in units of energy, and is similar to the more familiar concept of the decay constant in radioactive decay. It is also positive. $N(t)$ must be proportional to the density of states, $\rho(t)$, which is calculated from the time-dependant wave-function. Thus we have:

$$N_0 e^{-\frac{\Gamma}{\hbar}t} = N(t) \sim \rho = |\Psi_a(t,\boldsymbol{r})|^2 = \left| \mathrm{e}^{-\frac{i}{\hbar}Et}\, \psi_a(\boldsymbol{r}) \right|^2$$

$$\therefore \sqrt{N_0} e^{-\frac{\Gamma}{2\hbar}t} \sim \mathrm{e}^{-\frac{i}{\hbar}Et}\, \psi_a(\boldsymbol{r})$$

$\psi_a(\boldsymbol{r})$ will also be of an exponential form, due to the nature of Schrödinger’s equation. Also, due to its attenuation, we can thus write:

$$\psi_a(\boldsymbol{r}) \sim \mathrm{e}^{\pm iK}, \qquad K \in \mathbb{R}$$

$$\therefore e^{-\frac{\Gamma}{2\hbar}t} \sim \mathrm{e}^{-\frac{i}{\hbar}Et} \mathrm{e}^{\pm iK}$$

$$\therefore -\frac{\Gamma}{2\hbar}t \sim -\frac{i}{\hbar}Et \pm iK$$

$$\therefore \frac{i}{\hbar}Et \sim \frac{\Gamma}{2\hbar}t \pm iK$$

$$\therefore E \sim -i\frac{\Gamma}{2} \mp \frac{i\hbar}{t} iK$$

$$\therefore E \sim \pm\frac{\hbar K}{t} - i\frac{\Gamma}{2}$$

$$\therefore E = \pm E_R - i\frac{\Gamma}{2}$$

We can thus conclude that the energy must be complex with a negative imaginary part for resonance states. To find these energies, we simply use this information together with the fact that $f_l^{(in)}(E) = 0$. The complex values of E with negative imaginary part such that the Jost equation becomes zero thus corresponds with the resonant states.

The real part of such a zero point will give the resonant state energy, and the imaginary part is related to the resonant width, Γ, also simply referred to as the "width". Since this is basically the decay constant, the half-life, the time it takes for a ensemble of resonant states to decay by half the initial value, can be calculated from Γ with the following:

$$T_{1/2} = \frac{\hbar \ln 2}{\Gamma}$$

The half-life is an indication of how long a resonant state will last before it decays; A resonant state with large width will thus not last long, while a resonant state with a small width will indeed last long.

2.4 The Way Forward

This rather lengthy introduction now enables us to quite easily achieve our goal, since we finally have all the tools required to attack the problem.

I will begin by finding a method to easily calculate the Jost equations. The actual system will then be introduced, and I will proceed by using said method to find the Jost equations for this system.

By making use of the mathematical programming software, *Maple*, the zero points, also called the spectral points, of $f_l^{(in)}(k)$, with $k^2 = \frac{2\mu E}{\hbar^2}$ (equation (13)), are found.

The Jost function is quite obviously dependant on E, but equally obviously this dependence is through k. Since k is dependant on the square of E, a problem arises: spectral points that are purely imaginary in the k plane become real in the E plane. There must be a distinction between these values, since the E values corresponding to purely imaginary k values do not represent true bound states, but states that are dubbed *virtual* states, since such energies cannot exist in a physical sense. This state is only possible for systems where $l = 0$, and exist where the attraction is small. Where the attraction is stronger, virtual states become bound states.

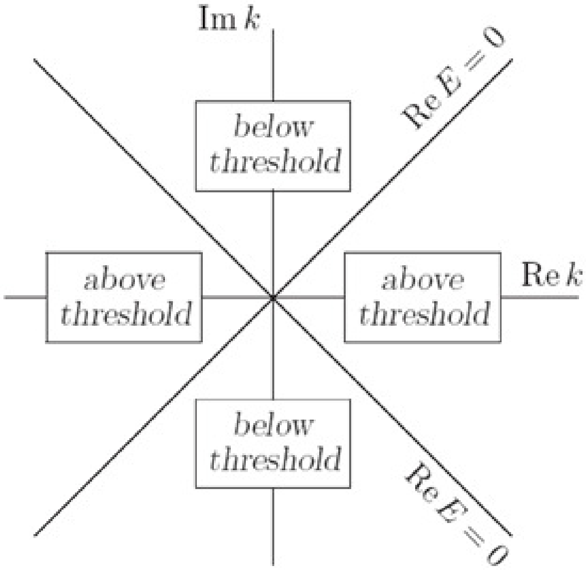


Figure 1

Also, resonances may be calculated in the E plane that cannot be considered true resonances, for the same reasons. These values are dubbed sub-threshold resonances, and can be seen as "virtual resonances", in a way. For our purposes, they are not important: they do not affect scattering, and behave in exactly the same way as resonances do. If we thus confuse a sub-threshold resonance with a true resonance, no harm is done. In the k plane, Figure 1 indicates where sub-threshold resonances would occur.

It is interesting to mention that, although true resonances and even sub-threshold resonances have negative imaginary part in the E-plane, each and every point has a mirror-image partner point relative to the real axis. Thus complex spectral points with positive imaginary parts exist, and correspond exactly with complex spectral points with negative imaginary part: both will have the same real value. This can be rigorously proven: see reference [1]. This symmetry also occurs in the k-plane, but around the imaginary k axis.

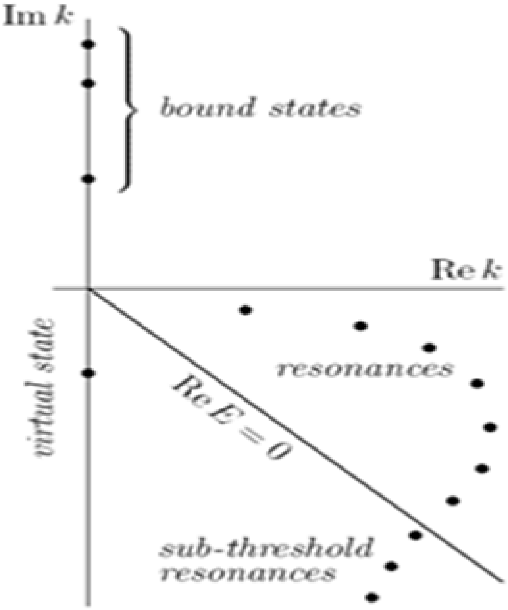


Figure 2

In this paper, I will find the spectral points of a system in the k-plane, and draw conclusions from this data. This is to avoid confusion with the virtual and sub-threshold states that cannot be distinguished from true bound and resonant states in the E plane. Also, since we are only interested in bound and resonant state dependence on the variables of the system, and not necessarily on the actual values of the energies, k-plane spectral points are more than suitable.

In the k-plane, purely imaginary positive spectral points will result in negative real points in the E

plane, which corresponds with bound states. Purely imaginary negative spectral points in the k-plane correspond with virtual states.

Complex spectral points with negative imaginary part and positive real part, as well as complex spectral points with positive imaginary part and negative real part, will correspond with resonance and sub threshold resonances. Since they have mirror images in the other quadrants, all complex spectral points are shown in the data, and are all pretty much thought of as resonant states, due to the symmetry. A plot of the spectral points for a typical system is shown in Figure 2.

Another highly important fact is that for a quantum mechanical system, there can be infinitely many resonant states, but there is a finite number of bound states. This can also be rigorously proven, and once again I refer the reader to reference [1]. A system might even have no bound states.

Using this information, much can be concluded from a set of data. First, we need to obtain this data, and we must thus be able to calculate the Jost equations. Of the pair, $f_l^{(in)}(E)$ appears to be the most useful for our purposes. As will be seen, $f_l^{(out)}(E)$ is of particular use in calculating $f_l^{(in)}(E)$, but after this is done, we do not need it any longer. It is of immense importance when considering scattering in a quantum mechanical system, and this is why it is also calculated.

3. Calculations

3.2 A Method to Calculate the Jost Equations

The most obvious way to calculate the Jost function would be to solve Schrödinger's equation in the region $r \to \infty$. Yet the whole point of using the Jost functions is to refrain from having to do so. Thus we must find an alternative way of calculating the Jost functions. Our starting point is equation (18), the radial time-independent Schrödinger's equation:

$$\left[\partial_r^2 + k^2 - \frac{l(l+1)}{r^2} - V(r)\right] u_l(r) = 0$$

We will find an alternative way of writing it that is more suitable for our needs. We start with the following:

$$\left[\partial_r^2 + k^2 - \frac{l(l+1)}{r^2}\right] u_l(r) = V(r)\, u_l(r) \tag{26}$$

The left hand side should look very familiar; it corresponds with the "free" redial equation, for which the solutions are known. The solution of the above thus takes the same form:

$$u_l(r) = F_l^{(in)}(E,r) h_l^{(-)}(kr) + F_l^{(out)}(E,r) h_l^{(+)}(kr) \tag{27}$$

Where $h_l^{(\pm)}(kr)$ once again represents the Riccati-Hankel functions, with the "+" indication the outgoing wave and the "–" indicating the incoming wave. $F_l^{(in/out)}(E,r)$ represents unknown functions, with the superscript indicating the correspondence with the incoming or outgoing wave. Note that for $r \to \infty$, (28) simply becomes the known equation (20):

$$u_l(r) = f_l^{(in)}(E) h_l^{(-)}(kr) + f_l^{(out)}(E) h_l^{(+)}(kr); \quad r \to \infty$$

With:

$$f_l^{(in)}(E) = \lim_{r\to\infty} F_l^{(in)}(E) \tag{28}$$

$$f_l^{(out)}(E) = \lim_{r\to\infty} F_l^{(out)}(E) \tag{29}$$

If we can thus calculate $F_l^{(in/out)}(E,r)$, we can calculate the Jost equations. We will apply the well-known Variation of Parameters method to solve (27), and thus introduce the Lagrange condition:

$$0 = \partial_r F_l^{(in)}(E,r) h_l^{(-)}(kr) + \partial_r F_l^{(out)}(E,r) h_l^{(+)}(kr) \tag{30}$$

This condition is arbitrary, and is allowed, since $F_l^{(in/out)}(E,r)$ must be dependent on each other in some way. Any condition relating the two equations would suffice, but this proves to be the most fruitful.

Now, take the first derivative of (28):

$$\partial_r u_l(r) = \left(\partial_r F_l^{(in)}(E,r) h_l^{(-)}(kr) + \partial_r F_l^{(out)}(E,r) h_l^{(+)}(kr)\right) + \left(F_l^{(in)}(E,r)\partial_r h_l^{(-)}(kr) + F_l^{(out)}(E,r)\partial_r h_l^{(+)}(kr)\right)$$

The first term disappears due to the Lagrange condition (31):

$$\therefore \partial_r u_l(r) = F_l^{(in)}(E,r)\partial_r h_l^{(-)}(kr) + F_l^{(out)}(E,r)\partial_r h_l^{(+)}(kr)$$

The derivative of the above, the second derivative of (28), is then:

$$\therefore \partial_r^2 u_l(r) = F_l^{(in)}(E,r)\partial_r^2 h_l^{(-)}(kr) + F_l^{(out)}(E,r)\partial_r^2 h_l^{(+)}(kr) + \partial_r F_l^{(in)}(E,r)\partial_r h_l^{(-)}(kr) + \partial_r F_l^{(out)}(E,r)\partial_r h_l^{(+)}(kr)$$

Consider (27):

$$\left[\partial_r^2 + k^2 - \frac{l(l+1)}{r^2}\right] u_l(r) = V(r)\, u_l(r)$$

$$\therefore \left[\ k^2 - \frac{l(l+1)}{r^2}\right] u_l(r) + \partial_r^2 u_l(r) = V(r)\, u_l(r)$$

Then substitute (28) and the expression for its second derivative into the above:

$$\therefore \left[\ k^2 - \frac{l(l+1)}{r^2} - V(r)\right]\left[F_l^{(in)}(E,r)h_l^{(-)}(kr) + \ F_l^{(out)}(E,r)h_l^{(+)}(kr)\right] + \left[F_l^{(in)}(E,r)\partial_r^2 h_l^{(-)}(kr) + F_l^{(out)}(E,r)\partial_r^2 h_l^{(+)}(kr) + \ \partial_r F_l^{(in)}(E,r)\partial_r h_l^{(-)}(kr) + \ \partial_r F_l^{(out)}(E,r)\partial_r h_l^{(+)}(kr)\right] = V(r)\, u_l(r)$$

$$\begin{aligned}\therefore \left[\ k^2 - \frac{l(l+1)}{r^2} - V(r)\right] F_l^{(in)}(E,r)h_l^{(-)}(kr) + \left[\ k^2 - \frac{l(l+1)}{r^2} - V(r)\right] F_l^{(out)}(E,r)h_l^{(+)}(kr) \\ + \left[F_l^{(in)}(E,r)\partial_r^2 h_l^{(-)}(kr) + \ F_l^{(out)}(E,r)\partial_r^2 h_l^{(+)}(kr) + \ \partial_r F_l^{(in)}(E,r)\partial_r h_l^{(-)}(kr) \right. \\ \left. + \ \partial_r F_l^{(out)}(E,r)\partial_r h_l^{(+)}(kr)\right] = V(r)\, u_l(r)\end{aligned}$$

$$\begin{aligned}\therefore \left\{\left[\ \partial_r^2 + k^2 - \frac{l(l+1)}{r^2} - V(r)\right] h_l^{(-)}(kr)\right\} F_l^{(in)}(E,r) \\ + \left\{\left[\partial_r^2 + \ k^2 - \frac{l(l+1)}{r^2} - V(r)\right] h_l^{(+)}(kr)\right\} F_l^{(out)}(E,r) \\ + \left[\ \partial_r F_l^{(in)}(E,r)\partial_r h_l^{(-)}(kr) + \ \partial_r F_l^{(out)}(E,r)\partial_r h_l^{(+)}(kr)\right] = V(r)\, u_l(r)\end{aligned}$$

But both $h_l^{(\pm)}(kr)$ are solutions to the “free” radial equation, which is represented in the first two terms. Thus both these terms will disappear:

$$\begin{aligned}\therefore \partial_r F_l^{(in)}(E,r)\partial_r h_l^{(-)}(kr) + \ \partial_r F_l^{(out)}(E,r)\partial_r h_l^{(+)}(kr) \\ = V(r)\left[F_l^{(in)}(E,r)h_l^{(-)}(kr) + \ F_l^{(out)}(E,r)h_l^{(+)}(kr)\right]\end{aligned} \tag{31}$$

The Lagrange condition (31) can be written in the following two ways:

$$\partial_r F_l^{(in)}(E,r) = -\ \partial_r F_l^{(out)}(E,r)\frac{h_l^{(+)}(kr)}{h_l^{(-)}(kr)} \tag{32}$$

$$\partial_r F_l^{(out)}(E,r) = -\partial_r F_l^{(in)}(E,r)\frac{h_l^{(-)}(kr)}{h_l^{(+)}(kr)} \tag{33}$$

If (32) is substituted into (31):

$$\begin{aligned}\therefore -\ \partial_r F_l^{(out)}(E,r)\frac{h_l^{(+)}(kr)}{h_l^{(-)}(kr)}\partial_r h_l^{(-)}(kr) + \ \partial_r F_l^{(out)}(E,r)\partial_r h_l^{(+)}(kr) \\ = V(r)\left[F_l^{(in)}(E,r)h_l^{(-)}(kr) + \ F_l^{(out)}(E,r)h_l^{(+)}(kr)\right]\end{aligned}$$

$$\begin{aligned}\therefore \partial_r F_l^{(out)}(E,r)\left[-\frac{h_l^{(+)}(kr)}{h_l^{(-)}(kr)}\partial_r h_l^{(-)}(kr) + \ \partial_r h_l^{(+)}(kr)\right] \\ = V(r)\left[F_l^{(in)}(E,r)h_l^{(-)}(kr) + \ F_l^{(out)}(E,r)h_l^{(+)}(kr)\right]\end{aligned}$$

We now multiply by $h_l^{(-)}(kr)$:

$$\begin{aligned}\therefore \partial_r F_l^{(out)}(E,r)\left[h_l^{(-)}(kr)\partial_r h_l^{(+)}(kr) - \ h_l^{(+)}(kr)\partial_r h_l^{(-)}(kr)\ \right] \\ = V(r)\, h_l^{(-)}(kr)\left[F_l^{(in)}(E,r)h_l^{(-)}(kr) + \ F_l^{(out)}(E,r)h_l^{(+)}(kr)\right]\end{aligned} \tag{34}$$

The expression:

$$h_l^{(-)}(kr)\partial_r h_l^{(+)}(kr) - h_l^{(+)}(kr)\partial_r h_l^{(-)}(kr)$$

Is the Wronskian of the Riccati-Hankel functions, and it is known from the theory of the Riccati-Hankel functions that it is equal to $2ik$. Thus (34) becomes:

$$\therefore \partial_r F_l^{(out)}(E,r) = \frac{1}{2ik}V(r)\, h_l^{(-)}(kr)\left[F_l^{(in)}(E,r)h_l^{(-)}(kr) + F_l^{(out)}(E,r)h_l^{(+)}(kr)\right]$$

In a similar fashion, when (33) is substituted into (31), the following is obtained:

$$\partial_r F_l^{(in)}(E,r) = -\frac{1}{2ik}V(r)\, h_l^{(+)}(kr)\left[\, F_l^{(in)}(E,r)h_l^{(-)}(kr) + F_l^{(out)}(E,r)h_l^{(+)}(kr)\,\right]$$

Thus we obtain a coupled set of equations:

$$\partial_r F_l^{(in)}(E,r) = -\frac{h_l^{(+)}(kr)}{2ik}V(r)\left[h_l^{(-)}(kr)\, F_l^{(in)}(E,r) + h_l^{(+)}(kr)\; F_l^{(out)}(E,r)\right] \tag{35}$$

$$\partial_r F_l^{(out)}(E,r) = +\frac{h_l^{(-)}(kr)}{2ik}V(r)\left[h_l^{(-)}(kr)\, F_l^{(in)}(E,r) + h_l^{(+)}(kr)\; F_l^{(out)}(E,r)\right] \tag{36}$$

This set of equations enables us to easily solve the problem of motion of a particle in a potential, and is equivalent to the time-independent Schrödinger's equation.

3.3 Calculating the Jost Equations

Firstly, we will assume $l = 0$. This is because, for most systems, the S-wave contribution is by far greater than the higher partial waves. S-wave contribution corresponds with $l = 0$.

The Riccati-Hankel functions then become:

$$h_0^{(+)}(kr) = -i\exp[+i\,kr\,] \tag{37}$$

$$h_0^{(-)}(kr) = +i\exp[-i\,kr\,] \tag{38}$$

Multiplying (38) and (39) then yields:

$$h_0^{(+)}(kr)\, h_0^{(-)}(kr) = \exp[+i\,kr - i\,kr\,]$$

$$\therefore\; h_0^{(+)}(kr)\, h_0^{(-)}(kr) = 1 \tag{39}$$

Also,

$$h_0^{(+)}(kr)\, h_0^{(+)}(kr) = -1\ \exp[+2\,i\,kr] \tag{40}$$

$$h_0^{(-)}(kr)\, h_0^{(-)}(kr) = -1\exp[-2\,ikr\,] \tag{41}$$

We can write (36) and (37) as follows:

$$\partial_r F_l^{(in)}(E,r) = -\frac{1}{2ik}V(r)\left[h_0^{(+)}(kr)\, h_0^{(-)}(kr)\, F_l^{(in)}(E,r) + h_0^{(+)}(kr)\, h_0^{(+)}(kr)\; F_0^{(out)}(E,r)\right]$$

$$\partial_r F_l^{(out)}(E,r) = +\frac{1}{2ik} V(r) \left[h_0^{(-)}(kr)\, h_0^{(-)}(kr)\, F_0^{(in)}(E,r) + \; h_0^{(-)}(kr)\, h_0^{(+)}(kr)\; F_0^{(out)}(E,r)\right]$$

The potential will be written as $V(r) = V$. $V(r)$ *is* dependant on r, but we consider V a constant in the general calculations, since we will be working with a step potential: when the region is specified, V will be adjusted accordingly.

We then substitute (40), (41) and (42) into the above to obtain the following:

$$\partial_r F_0^{(in)}(E,r) = -\frac{1}{2ik} V \left[\, F_0^{(in)}(E,r) - \exp[+\,2\,i\,kr\;] \;\; F_0^{(out)}(E,r)\right] \qquad (42)$$

$$\partial_r F_0^{(out)}(E,r) = +\frac{1}{2ik} V \left[-\exp[-\,2\,i\,kr\;]\, F_0^{(in)}(E,r) + \; F_0^{(out)}(E,r)\right] \qquad (43)$$

Rearrange (42) to make $F_0^{(out)}(E,r)$ the subject of the formula:

$$\partial_r F_0^{(in)}(E,r) = -\frac{1}{2ik} V \left[\, F_0^{(in)}(E,r) - \exp[+\,2\,i\,kr\;] \;\; F_0^{(out)}(E,r)\right]$$

$$\therefore -\frac{2ik}{V}\; \partial_r F_0^{(in)}(E,r) = \; F_0^{(in)}(E,r) - \; \exp[+\,2\,i\,kr] \;\; F_0^{(out)}(E,r)$$

$$\therefore \exp[+\,2\,i\,kr\;] \;\; F_0^{(out)}(E,r) \; = + \; \frac{2ik}{V}\; \partial_r F_0^{(in)}(E,r) + \; F_0^{(in)}(E,r)$$

$$\therefore F_0^{(out)}(E,r) \; = \left[\frac{2ik}{V}\; \partial_r F_0^{(in)}(E,r) + \; F_0^{(in)}(E,r)\right] \exp[-\,2\,i\,kr\,] \qquad (44)$$

Take the derivative of (44):

$$\begin{aligned} \partial_r\, F_0^{(out)}(E,r) \; &= \left[\frac{2ik}{V}\; \partial_r^2 F_0^{(in)}(E,r) + \partial_r\, F_0^{(in)}(E,r)\right] \exp[-\,2\,i\,kr] \\ &\quad - 2ik \left[\frac{2ik}{V}\; \partial_r F_0^{(in)}(E,r) + \; F_0^{(in)}(E,r)\right] \exp[-\,2\,i\,kr\,] \end{aligned}$$

$$\begin{aligned} &\therefore \partial_r\, F_0^{(out)}(E,r) \\ &\qquad = \left\{\frac{2ik}{V}\; \partial_r^2 F_0^{(in)}(E,r) + \left[1 - \frac{(2ik)^2}{V}\right] \partial_r\, F_0^{(in)}(E,r) \right. \\ &\qquad\quad \left. - \,2ik\, F_0^{(in)}(E,r)\right\} \exp[-\,2\,i\,kr\;] \end{aligned} \qquad (45)$$

Substitute (44) into (43):

$$\therefore \partial_r F_0^{(out)}(E,r) = +\frac{1}{2ik} V \left[-\,F_0^{(in)}(E,r) + \frac{2ik}{V}\; \partial_r F_0^{(in)}(E,r) + \; F_0^{(in)}(E,r)\right] \exp[-\,2\,i\,kr\;]$$

$$\therefore \partial_r F_0^{(out)}(E,r) = \;\; \partial_r F_0^{(in)}(E,r) \exp[-\,2\,i\,kr\;]$$

Now substitute (45) into this expression:

$$\therefore \left\{\frac{2ik}{V}\,\partial_r^2 F_0^{(in)}(E,r) + \left[1 - \frac{(2ik)^2}{V}\right]\partial_r\, F_0^{(in)}(E,r) - 2ik\, F_0^{(in)}(E,r)\right\}\exp[-2\,i\,kr\,]$$
$$= \partial_r F_0^{(in)}(E,r)\exp[-2\,i\,kr\,]$$

Note that the exponentials cancel:

$$\therefore \left\{\frac{2ik}{V}\,\partial_r^2 F_0^{(in)}(E,r) + \left[1 - \frac{(2ik)^2}{V}\right]\partial_r\, F_0^{(in)}(E,r) - 2ik\, F_0^{(in)}(E,r)\right\} = \partial_r F_0^{(in)}(E,r)$$

$$\therefore \frac{2ik}{V}\,\partial_r^2 F_0^{(in)}(E,r) - \frac{(2ik)^2}{V}\,\partial_r\, F_0^{(in)}(E,r) - 2ik\, F_0^{(in)}(E,r) = 0$$

$$\therefore\ \partial_r^2 F_0^{(in)}(E,r) - 2ik\,\partial_r\, F_0^{(in)}(E,r) - V\, F_0^{(in)}(E,r) = 0 \qquad (46)$$

We need to solve this differential equation. Suppose the solution is of the form:

$$F_l^{(in)}(E,r) = e^{\lambda r}$$

Thus we can write:

$$\therefore\ \partial_r F_l^{(in)}(E,r) = \lambda\, e^{\lambda r}$$

$$\therefore\ \partial_r^2 F_l^{(in)}(E,r) = \lambda^2\, e^{\lambda r}$$

Substituting these three equations into the differential equation (46) yields:

$$\lambda^2\, e^{\lambda r} - 2ik\,\lambda\, e^{\lambda r} - Ve^{\lambda r} = 0$$

$$\therefore\ \lambda^2 - 2ik\,\lambda - V = 0$$

Now we need to find the solutions of λ:

$$\lambda = \frac{2ik \pm \sqrt{(2ik)^2 + 4V}}{2}$$

$$\therefore \lambda = \frac{2ik \pm \sqrt{-4k^2 + 4V}}{2}$$

$$\therefore \lambda = \frac{2ik \pm 2\sqrt{V - k^2}}{2}$$

$$\therefore \lambda = ik \pm \sqrt{V - k^2}$$

$$\therefore \lambda = ik \pm i\sqrt{k^2 - V}$$

Let:

$$K = \sqrt{k^2 - V} \qquad (47)$$

$$\therefore \lambda = (k \pm K)i$$

The solution to the differential equation is thus a linear combination of the proposed solution with the possible values of λ:

$$F_0^{(in)}(E,r) = P1\, e^{(k-\,K)ir} \;+\; P2\, e^{(k+\,K)ir} \tag{48}$$

$P1$ and $P2$ are constants. Now we need to find $F_0^{(out)}(E,r)$. We take the derivative of our expression for $F_0^{(in)}(E,r)$:

$$\therefore\, \partial_r F_0^{(in)}(E,r) = (k-\,K)iP1\, e^{(k-\,K)ir} \;+\; (k+\,K)iP2\, e^{(k+\,K)ir} \tag{49}$$

We substitute (48) and (49) into (50):

$$F_0^{(out)}(E,r) \;= \left[\frac{2ik}{V}\,\partial_r F_0^{(in)}(E,r) + F_0^{(in)}(E,r)\right] \exp[-\,2\,i\,kr\,]$$

$$F_0^{(out)}(E,r) \;= \Bigg[\frac{2ik}{V}(k-\,K)iP1\, e^{(k-\,K)ir} \;+\; \frac{2ik}{V}(k+\,K)iP2\, e^{(k+\,K)ir} + P1\, e^{(k-\,K)ir} \;+\; P2\, e^{(k+\,K)ir}\Bigg] \exp[-\,2\,i\,kr\,]$$

$$\therefore\; F_0^{(out)}(E,r) = \left[\left(-\frac{2k^2}{V} + K\frac{2k}{V}\right)P1\, e^{(k-\,K)ir} \;+\; \left(-k\frac{2k^2}{V} - K\frac{2k}{V}\right)P2\, e^{(k+\,K)ir} + P1\, e^{(k-\,K)ir} \;+\; P2\, e^{(k+\,K)ir}\right] \exp[-\,2\,i\,kr\,]$$

$$\therefore\; F_0^{(out)}(E,r) \;= \left(1 - \frac{2k^2}{V} + \frac{2k}{V}K\right)P1\, e^{(-k-\,K)ir} \;+\; \left(1 - \frac{2k^2}{V} - \frac{2k}{V}K\right)P2\, e^{(-k+\,K)ir}$$

So finally we have:

$$F_0^{(in)}(E,r) = P1\, e^{(k-\,K)ir} \;+\; P2\, e^{(k+\,K)ir} \tag{50}$$

$$F_0^{(out)}(E,r) \;= \left(1 - \frac{2k^2}{V} + \frac{2k}{V}K\right)P1\, e^{(-k-\,K)ir} + \left(1 - \frac{2k^2}{V} - \frac{2k}{V}K\right)P2\, e^{(-k+\,K)ir} \tag{51}$$

All that remain is to find the constants $P1$ and $P2$, that are determined with the boundary conditions. (50) and (51) are thus general solutions for any step-potential. Once $P1$ and $P2$ are determined, we take the limit of (50) and (51) as $r \to \infty$, as indicated in (28) and (29), to obtain the Jost functions.

3.4 The Jost Equations for the Given Potential

3.4.1 The Potential

Finally, the preliminaries have been attended to, and we will apply all our calculations to the potential shown in Figure 3.

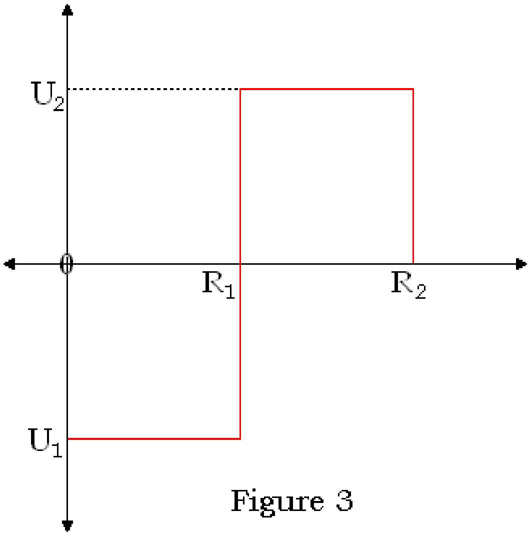


Figure 3

$$U(r) = \begin{cases} U_1 & if \quad 0 < r < R_1 \\ U_2 & if \quad R_1 < r < R_2 \\ 0 & if \quad R_2 < r < \infty \end{cases} \tag{52}$$

Recall equation (14):

$$V(r) = \frac{2\mu}{\hbar^2} U(r)$$

$$\therefore V(r) = \begin{cases} \frac{2\mu}{\hbar^2} U_1 & if \quad 0 < r < R_1 \\ \frac{2\mu}{\hbar^2} U_2 & if \quad R_1 < r < R_2 \\ 0 & if \quad R_2 < r < \infty \end{cases}$$

It should now become clear why we assumed that $V(r) = V$ in the calculations. We will simply let:

$$V = \begin{cases} V_1 & if \quad 0 < r < R_1 \\ V_2 & if \quad R_1 < r < R_2 \\ 0 & if \quad R_2 < r < \infty \end{cases} \tag{53}$$

With:

$$V_{1,2} = \frac{2\mu}{\hbar^2} U_{1,2}$$

It should also be clear that the wave function will differ in each of the three regions of Figure 3, due to the difference in potential in each region. Thus the functions $F_l^{(in)}(E,r)$ and $F_l^{(out)}(E,r)$ will also differ in the three regions, which implies that the constants $P1$ and $P2$ also differ in each region, since the boundaries of each region differ. Unfortunately the constant values for the first two regions are required to calculate the constants for the third region, the region we are most interested in: the limit of $F_l^{(in)}(E,r)$ and $F_l^{(out)}(E,r)$ as $r \to \infty$ falls within this region.

It is relatively easy to calculate the constants for the first region, since the wave equation behaves in a very specific way at $r = 0$.

In the second and third region, we make use of the fact that that the wave function and its derivative with respect to r must be continuous for all values of r, implying that the same holds for $\psi_a(\boldsymbol{r})$, which in turn implies the same for $u_l(E,r)$. This arises from the fact that, as is known from Calculus, if two functions are continuous in a specific interval, the product of these two functions will also be continuous in this interval. Thus $u_0(E,r)$and $\partial_r u_0(E,r)$ are continuous at $r = R_1$ and $r = R_2$.

To simplify matters, we consider each region separately.

3.4.2 Region One: $0 < r < R_1$

We then have the following:

$$P1 = P1_1$$

$$P2 = P2_1$$

$$V = V_1$$

$$K = K_1 = \sqrt{k^2 - V_1}$$

$$F_{01}^{(in)}(E,r) = P1_1\, e^{(k - K_1)ir} + P2_1 e^{(k + K_1)ir} \tag{54}$$

$$\begin{aligned} F_{01}^{(out)}(E,r) &= \left(1 - \frac{2k^2}{V_1} + \frac{2k}{V_1}K_1\right) P1_1\, e^{(-k - K_1)ir} \\ &\quad + \left(1 - \frac{2k^2}{V_1} - \frac{2k}{V_1}K_1\right) P2_1\, e^{(-k + K_1)ir} \end{aligned} \tag{55}$$

The added subscripts are indicative of the applicable region. The solution to the Radial Schrödinger's Equation for this region is then given by:

$$u_{01}(E,r) = F_{01}^{(in)}(E,r)\, h_0^{(-)}(kr) + F_{01}^{(out)}(E,r)\, h_0^{(+)}(kr)$$

As is discussed earlier, we know that $u_l(E,0) = 0$. Let us apply this condition to the above:

$$u_{01}(E,0) = F1_0^{(in)}(E,0)\, h_0^{(-)}(0) + F1_0^{(out)}(E,0)\, h_0^{(+)}(0) = 0$$

$$\therefore F1_0^{(in)}(E,0)\, i + F1_0^{(out)}(E,0)(-i) = 0$$

$$\therefore F1_0^{(in)}(E,0) = F1_0^{(out)}(E,0) \tag{56}$$

From the alternative Schrödinger's Radial Equation, equations (35) and (36):

$$\partial_r F_0^{(in)}(E,0) = -\frac{h_0^{(+)}(k0)}{2ik} V(0) \left[h_0^{(-)}(k0)\, F_0^{(in)}(E,0) + h_0^{(+)}(k0)\ F_0^{(out)}(E,0)\right]$$

$$\partial_r F_0^{(out)}(E,r) = +\frac{h_0^{(-)}(k0)}{2ik} V(0) \left[h_0^{(-)}(k0)\, F_0^{(in)}(E,0) + h_0^{(+)}(k0)\ F_0^{(out)}(E,0)\right]$$

Taking (56) into account:

$$\therefore \partial_r F1_l^{(in)}(E,0) = -\frac{(-i)}{2ik} V_1 \left[i\, F1_0^{(in)}(E,r) + (-i)\ F1_0^{(in)}(E,0)\right] = 0$$

$$\partial_r F1_l^{(out)}(E,0) = +\frac{i}{2ik} V_1 \left[i\, F1_0^{(in)}(E,r) + (-i)\ F1_0^{(in)}(E,0)\right] = 0$$

Thus we obtain:

$$\partial_r F1_0^{(in)}(E,0) = \partial_r F1_0^{(out)}(E,0) = 0$$

Thus $F1_0^{(in)}(E,0)$ and $F1_0^{(out)}(E,0)$ are both constants, and from (56) they must be equal:

$$F1_0^{(in)}(E,0) = F1_0^{(out)}(E,0) = constant$$

We are not concerned with the normalization of these functions, so we let this constant value equal 1. Thus:

$$F1_0^{(in/out)}(E,0) = 1 \tag{57}$$

Applying this to (54) is easy:

$$F_{01}^{(in)}(E,0) = P1_1 + P2_1 = 1$$

$$\therefore P2_1 = P1_1 - 1 \tag{58}$$

Applying it to (55) is more challenging. Consider:

$$F_{01}^{(out)}(E,0) = \left(1 - \frac{2k^2}{V_1} + \frac{2k}{V_1} K_1\right) P1_1 + \left(1 - \frac{2k^2}{V_1} - \frac{2k}{V_1} K_1\right) P2_1$$

Substitute (58):

$$F_{01}^{(out)}(E,0) = \left(1 - \frac{2k^2}{V_1} + \frac{2k}{V_1}K_1\right)P1_1 + \left(1 - \frac{2k^2}{V_1} - \frac{2k}{V_1}K_1\right)(P1_1 - 1)$$

$$F_{01}^{(out)}(E,0) = \left(\left(1 - \frac{2k^2}{V_1}\right) + \frac{2k}{V_1}K_1\right)P1_1 + \left(\left(1 - \frac{2k^2}{V_1}\right) - \frac{2k}{V_1}K_1\right)P1_1 - \left(1 - \frac{2k^2}{V_1} - \frac{2k}{V_1}K_1\right)$$

$$\therefore F_{01}^{(out)}(E,0) = 2\left(1 - \frac{2k^2}{V_1}\right)P1_1 - \left(1 - \frac{2k^2}{V_1} - \frac{2k}{V_1}K_1\right)$$

Now apply (57):

$$2\left(1 - \frac{2k^2}{V_1}\right)P1_1 - \left(1 - \frac{2k^2}{V_1} - \frac{2k}{V_1}K_1\right) = 1$$

$$\therefore P1_1 = \frac{\left(1 - \frac{2k^2}{V_1} - \frac{2k}{V_1}K_1\right)}{2\left(1 - \frac{2k^2}{V_1}\right)}$$

$$\therefore P1_1 = \frac{(V_1 - 2k^2) - 2k\,K_1}{2(V_1 - 2k^2)}$$

$$\therefore P1_1 = \frac{1}{2} - \frac{k\,K_1}{V_1 - 2k^2}$$

To find $P2_1$ we simply use (58):

$$P2_1 = 1 - P1_1$$

$$\therefore P2_1 = 1 - P1_1 = 1 - \frac{(V_1 - 2k^2) - 2k\,K_1}{2(V_1 - 2k^2)}$$

$$\therefore P2_1 = \frac{(V_1 - 2k^2) + 2k\,K_1}{2(V_1 - 2k^2)}$$

$$\therefore P2_1 = \frac{1}{2} + \frac{k\,K_1}{V_1 - 2k^2}$$

To sum up:

$$P1_1 = \frac{1}{2} - \frac{k\,K_1}{V_1 - 2k^2} \tag{59}$$

$$P2_1 = \frac{1}{2} + \frac{k\,K_1}{V_1 - 2k^2} \tag{60}$$

3.4.3 Region Two: $R_1 < r < R_2$

We then have the following:

$$P1 = P1_2$$

$$P2 = P2_2$$

$$V = V_2$$

$$K = K_2 = \sqrt{k^2 - V_2}$$

$$F_{02}^{(in)}(E,r) = P1_2\, e^{(k - K_2)ir} + P2_2 e^{(k + K_2)ir} \tag{61}$$

$$\begin{aligned} F_{02}^{(out)}(E,r) &= \left(1 - \frac{2k^2}{V_2} + \frac{2k}{V_2}K_2\right) P1_2\, e^{(-k - K_2)ir} \\ &+ \left(1 - \frac{2k^2}{V_2} - \frac{2k}{V_2}K_2\right) P2_2\, e^{(-k + K_2)ir} \end{aligned} \tag{62}$$

$$u_{02}(E,r) = F_{02}^{(in)}(E,r)\, h_0^{(-)}(kr) + F_{02}^{(out)}(E,r)\, h_0^{(+)}(kr)$$

We know that:

$$u_{01}(E,R_1) = u_{02}(E,R_1)$$

$$\begin{aligned} \therefore F_{01}^{(in)}(E,R_1)\, h_0^{(-)}(kR_1) + F_{01}^{(out)}(E,R_1)\, h_0^{(+)}(kR_1) \\ = F_{02}^{(in)}(E,R_1)\, h_0^{(-)}(kR_1) + F_{02}^{(out)}(E,R_1)\, h_0^{(+)}(kR_1) \end{aligned}$$

$$\therefore F_{01}^{(in)}(E,R_1)\, i\, \mathrm{e}^{-\,i\,kR_1} - F_{01}^{(out)}(E,R_1) i\, \mathrm{e}^{+\,i\,kR_1} = F_{02}^{(in)}(E,R_1)\, i\, \mathrm{e}^{-\,i\,kR_1} - F_{02}^{(out)}(E,R_1) i\, \mathrm{e}^{+\,i\,kR_1}$$

$$\begin{aligned} \therefore F_{01}^{(in)}(E,R_1)\ \mathrm{e}^{-\,i\,kR_1} - F_{02}^{(in)}(E,R_1)\ \mathrm{e}^{-\,i\,kR_1} \\ = F_{01}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1} - F_{02}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1} \end{aligned} \tag{63}$$

We also know that:

$$\partial_r u_{01}(E,R_1) = \partial_r u_{02}(E,R_1)$$

$$\begin{aligned} \therefore \partial_{r=R_1}\left(F_{01}^{(in)}(E,r)\, h_0^{(-)}(kr) + F_{01}^{(out)}(E,r)\, h_0^{(+)}(kr)\right) \\ = \partial_{r=R_1}\left(F_{02}^{(in)}(E,r)\, h_0^{(-)}(kr) + F_{02}^{(out)}(E,r)\, h_0^{(+)}(kr)\right) \end{aligned}$$

$$\begin{aligned} \therefore \partial_{r=R_1}\left(F_{01}^{(in)}(E,r)\, i\, \mathrm{e}^{-\,i\,kr} - F_{01}^{(out)}(E,r) i\, \mathrm{e}^{+\,i\,kr}\right) \\ = \partial_{r=R_1}\left(F_{02}^{(in)}(E,r)\, i\, \mathrm{e}^{-\,i\,kr} - F_{02}^{(out)}(E,r) i\, \mathrm{e}^{+\,i\,kr}\right) \end{aligned}$$

$$\begin{aligned} \therefore \partial_{r=R_1}\left(F_{01}^{(in)}(E,r)\ \mathrm{e}^{-\,i\,kr} - F_{01}^{(out)}(E,r)\, \mathrm{e}^{+\,i\,kr}\right) \\ = \partial_{r=R_1}\left(F_{02}^{(in)}(E,r)\, \mathrm{e}^{-\,i\,kr} - F_{02}^{(out)}(E,r)\, \mathrm{e}^{+\,i\,kr}\right) \end{aligned}$$

$$\begin{aligned}\therefore &\left(-ik\, F_{01}^{(in)}(E,R_1)\ \mathrm{e}^{-\,i\,kR_1} - ik\, F_{01}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1}\right)\\ &+\left(\,\partial_r F_{01}^{(in)}(E,R_1)\ \mathrm{e}^{-\,i\,kR_1} - \partial_r F_{01}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1}\right)\\ &=\left(-ik\, F_{02}^{(in)}(E,R_1)\, \mathrm{e}^{-\,i\,kR_1} - ik\, F_{02}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1}\right)\\ &+\left(\,\partial_r F_{02}^{(in)}(E,R_1)\, \mathrm{e}^{-\,i\,kR_1} - \,\partial_r F_{02}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1}\right)\end{aligned} \qquad (64)$$

Consider the two equations (42) and (43) which are derived from (35) and (36):

$$\partial_r F_0^{(in)}(E,r) = -\frac{1}{2ik} V \left[\, F_0^{(in)}(E,r) - \mathrm{e}^{+\,2\,i\,kr}\ F_0^{(out)}(E,r)\right]$$

$$\partial_r F_0^{(out)}(E,r) = +\frac{1}{2ik} V \left[-\mathrm{e}^{-\,2\,i\,kr}\, F_0^{(in)}(E,r) + \ F_0^{(out)}(E,r)\right]$$

$$\begin{aligned}\therefore\ &\partial_r F_0^{(in)}(E,r)\mathrm{e}^{-\,i\,kr} - \partial_r F_0^{(out)}(E,r)\mathrm{e}^{+\,i\,kr}\\ &= -\frac{1}{2ik} V \left[\, \mathrm{e}^{-\,i\,kr} F_0^{(in)}(E,r) - \mathrm{e}^{+\,i\,kr}\ \ F_0^{(out)}(E,r)\right]\\ &- \frac{1}{2ik} V \left[-\mathrm{e}^{-\,i\,kr}\ F_0^{(in)}(E,r) + \mathrm{e}^{+\,i\,kr}\, F_0^{(out)}(E,r)\right]\end{aligned}$$

$$\begin{aligned}\therefore\ &\partial_r F_0^{(in)}(E,r)\mathrm{e}^{-\,i\,kr} - \partial_r F_0^{(out)}(E,r)\mathrm{e}^{+\,i\,kr}\\ &= -\frac{1}{2ik} V \Big[\, \mathrm{e}^{-\,i\,kr} F_0^{(in)}(E,r) - \mathrm{e}^{+\,i\,kr}\ \ F_0^{(out)}(E,r) - \mathrm{e}^{-\,i\,kr}\, F_0^{(in)}(E,r)\\ &+ \mathrm{e}^{+\,i\,kr}\, F_0^{(out)}(E,r)\Big]\end{aligned}$$

$$\therefore\ \partial_r F_0^{(in)}(E,r)\mathrm{e}^{-\,i\,kr} - \partial_r F_0^{(out)}(E,r)\mathrm{e}^{+\,i\,kr} = 0$$

$$\therefore\ \partial_r F_{01/2}^{(in)}(E,R_1)\mathrm{e}^{-\,i\,kR_1} - \partial_r F_{01/2}^{(out)}(E,R_1)\mathrm{e}^{+\,i\,kR_1} = 0$$

Taking this into account, (64) becomes:

$$\begin{aligned}&\left(-ik\, F_{01}^{(in)}(E,R_1)\ \mathrm{e}^{-\,i\,kR_1} - ik\, F_{01}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1}\right)\\ &= \left(-ik\, F_{02}^{(in)}(E,R_1)\, \mathrm{e}^{-\,i\,kR_1} - ik\, F_{02}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1}\right)\end{aligned}$$

$$\therefore\ F_{01}^{(in)}(E,R_1)\ \mathrm{e}^{-\,i\,kR_1} - \ F_{02}^{(in)}(E,R_1)\, \mathrm{e}^{-\,i\,kR_1} = -\,F_{01}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1} + \ F_{02}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1}$$

Now substitute (63):

$$F_{01}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1} - \ F_{02}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1} = -\,F_{01}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1} + \ F_{02}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1}$$

$$\therefore\ F_{01}^{(out)}(E,R_1)\ =\ F_{02}^{(out)}(E,R_1)$$

When substituting this back into (63) we obtain:

$$F_{01}^{(in)}(E,R_1)\ \mathrm{e}^{-\,i\,kR_1} - \ F_{02}^{(in)}(E,R_1)\ \mathrm{e}^{-\,i\,kR_1} = F_{01}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1} - F_{01}^{(out)}(E,R_1)\, \mathrm{e}^{+\,i\,kR_1}$$

$$\therefore\ F_{01}^{(in)}(E,R_1)\ \mathrm{e}^{-\,i\,kR_1} - \ F_{02}^{(in)}(E,R_1)\ \mathrm{e}^{-\,i\,kR_1} = 0$$

$$\therefore F_{01}^{(in)}(E,R_1) \;=\; F_{02}^{(in)}(E,R_1)$$

We then have the following highly useful result:

$$F_{01}^{(in)}(E,R_1) \;=\; F_{02}^{(in)}(E,R_1) \tag{65}$$

$$F_{01}^{(out)}(E,R_1) \;=\; F_{02}^{(out)}(E,R_1) \tag{66}$$

In fact, this is valid for $r = R_2$ as well, which can be shown in an identical way to the above. For this reason, the derivation is not shown but assumed to be true.

From (65) we can then write:

$$P1_1\, e^{(k-\,K_1)iR_1} \;+\; P2_1 e^{(k+\,K_1)iR_1} = P1_2\, e^{(k-\,K_2)iR_1} \;+\; P2_2 e^{(k+\,K_2)iR_1}$$

$$\therefore P1_1\, e^{(k-\,K_1)iR_1} \;+\; P2_1 e^{(k+\,K_1)iR_1} -\; P1_2\, e^{(k-\,K_2)iR_1} \;=\; +P2_2 e^{(k+\,K_2)iR_1}$$

$$\therefore\; P2_2 = \;P1_1\, e^{(-\,K_1-K_2)iR_1} \;+\; P2_1 e^{(+\,K_1-K_2)iR_1} -\; P1_2\, e^{(-2\,K_2)iR_1} \tag{67}$$

From (66) we have:

$$\begin{aligned}\left(1-\frac{2k^2}{V_1}+\frac{2k}{V_1}K_1\right)P1_1\, e^{(-k-\,K_1)iR_1} &+ \left(1-\frac{2k^2}{V_1}-\frac{2k}{V_1}K_1\right)P2_1\, e^{(-k+\,K_1)iR_1} \\ &= \left(1-\frac{2k^2}{V_2}+\frac{2k}{V_2}K_2\right)P1_2\, e^{(-k-\,K_2)iR_1} + \left(1-\frac{2k^2}{V_2}-\frac{2k}{V_2}K_2\right)P2_2\, e^{(-k+\,K_2)iR_1}\end{aligned}$$

Multiply by $V_1V_2\, e^{kiR_1}$:

$$\begin{aligned}\therefore (V_1V_2-2k^2V_2+2kV_2K_1)P1_1\, e^{(-\,K_1)iR_1} &+ (V_1V_2-2k^2V_2-\;2kV_2K_1)P2_1\, e^{(+\,K_1)iR_1} \\ &= (V_1V_2-2k^2V_1+2kV_1K_2)P1_2\, e^{(-\,K_2)iR_1} \\ &+ (V_1V_2-2k^2V_1-\;2kV_1K_2)P2_2\, e^{(+\,K_2)iR_1}\end{aligned}$$

Now substitute (67):

$$\begin{aligned}\therefore (V_1V_2-2k^2V_2+2kV_2K_1)P1_1\, e^{(-\,K_1)iR_1} &+ (V_1V_2-2k^2V_2-\;2kV_2K_1)P2_1\, e^{(+\,K_1)iR_1} \\ &= (V_1V_2-2k^2V_1+2kV_1K_2)P1_2\, e^{(-\,K_2)iR_1} \\ &+ (V_1V_2-2k^2V_1-\;2kV_1K_2)\big(P1_1\, e^{(-\,K_1-K_2)iR_1} + P2_1 e^{(+\,K_1-K_2)iR_1} \\ &- P1_2\, e^{(-2\,K_2)iR_1}\big)\, e^{(+\,K_2)iR_1}\end{aligned}$$

$$\begin{aligned}\therefore (V_1V_2-2k^2V_2+2kV_2K_1)P1_1\, e^{(-\,K_1)iR_1} &+ (V_1V_2-2k^2V_2-\;2kV_2K_1)P2_1\, e^{(+\,K_1)iR_1} \\ &= (V_1V_2-2k^2V_1+2kV_1K_2)P1_2\, e^{(-\,K_2)iR_1} \\ &+ (V_1V_2-2k^2V_1-\;2kV_1K_2)\big(P1_1\, e^{(-\,K_1)iR_1} + P2_1 e^{(+\,K_1)iR_1} -\; P1_2\, e^{(-\,K_2)iR_1}\big)\end{aligned}$$

$$\begin{aligned}
\therefore (V_1V_2 - 2k^2V_2 + 2kV_2K_1)P1_1\, e^{(-\,K_1)iR_1} &+ (V_1V_2 - 2k^2V_2 - 2kV_2K_1)P2_1\, e^{(+\,K_1)iR_1} \\
&= (V_1V_2 - 2k^2V_1 + 2kV_1K_2)P1_2\, e^{(-\,K_2)iR_1} \\
&+ (V_1V_2 - 2k^2V_1 - 2kV_1K_2)P1_1\, e^{(-\,K_1)iR_1} \\
&+ (V_1V_2 - 2k^2V_1 - 2kV_1K_2)P2_1 e^{(+\,K_1)iR_1} \\
&- (V_1V_2 - 2k^2V_1 - 2kV_1K_2)P1_2\, e^{(-\,K_2)iR_1}
\end{aligned}$$

$$\begin{aligned}
\therefore (-2k^2V_2 + 2kV_2K_1 + 2k^2V_1 + 2kV_1K_2)P1_1\, e^{(-\,K_1)iR_1} \\
+ (-2k^2V_2 - 2kV_2K_1 + 2k^2V_1 + 2kV_1K_2)P2_1\, e^{(+\,K_1)iR_1} \\
= (4kV_1K_2)P1_2\, e^{(-\,K_2)iR_1}
\end{aligned}$$

Multiply by $\frac{1}{2k} e^{(+\,K_2)iR_1}$:

$$\begin{aligned}
\therefore (-kV_2 + V_2K_1 + kV_1 + V_1K_2)P1_1\, e^{(-\,K_1+\,K_2)iR_1} \\
+ (-kV_2 - V_2K_1 + kV_1 + V_1K_2)P2_1\, e^{(+\,K_1+\,K_2)iR_1} = 2\,V_1K_2P1_2
\end{aligned}$$

$$\therefore \frac{(k(V_1 - V_2) + V_1K_2 + V_2K_1)P1_1\, e^{(-\,K_1+\,K_2)iR_1} + (k(V_1 - V_2) + V_1K_2 - V_2K_1)P2_1\, e^{(+\,K_1+\,K_2)iR_1}}{2\,V_1K_2}$$

$$= P1_2$$

$$\begin{aligned}
\therefore P1_2 = \frac{1}{2}\left(\frac{k(V_1 - V_2)}{V_1K_2} + 1 + \frac{V_2K_1}{V_1K_2}\right) P1_1\, e^{(-\,K_1+\,K_2)iR_1} \\
+ \frac{1}{2}\left(\frac{k(V_1 - V_2)}{V_1K_2} + 1 - \frac{V_2K_1}{V_1K_2}\right) P2_1\, e^{(+\,K_1+\,K_2)iR_1}
\end{aligned}$$

$$\begin{aligned}
\therefore P1_2 = \frac{1}{2\,V_1K_2}(kV_1 - kV_2 + V_1K_2 + V_2K_1)P1_1\, e^{(-\,K_1+\,K_2)iR_1} \\
+ \frac{1}{2\,V_1K_2}(kV_1 - kV_2 + V_1K_2 - V_2K_1)P2_1\, e^{(+\,K_1+\,K_2)iR_1}
\end{aligned}$$

$$\begin{aligned}
\therefore P1_2 = \frac{1}{2\,V_1K_2}\big(V_1(\,K_2 + k) + V_2(K_1 - k)\big)P1_1\, e^{(-\,K_1+\,K_2)iR_1} \\
+ \frac{1}{2\,V_1K_2}\big(V_1(K_2 + k) + V_2(-K_1 - k)\big)P2_1\, e^{(+\,K_1+\,K_2)iR_1}
\end{aligned}$$

Now we substitute this into our expression for $P2_2$, equation (67):

$$P2_2 = P1_1\, e^{(-\,K_1-K_2)iR_1} + P2_1 e^{(+\,K_1-K_2)iR_1} - P1_2\, e^{(-2\,K_2)iR_1}$$

$$\begin{aligned}
\therefore P2_2 = P1_1\, e^{(-\,K_1-K_2)iR_1} + P2_1 e^{(+\,K_1-K_2)iR_1} \\
- \Bigg(\frac{1}{2\,V_1K_2}\big(V_1(\,K_2 + k) + V_2(K_1 - k)\big)P1_1\, e^{(-\,K_1+\,K_2)iR_1} \\
+ \frac{1}{2\,V_1K_2}\big(V_1(K_2 + k) + V_2(-K_1 - k)\big)P2_1\, e^{(+\,K_1+\,K_2)iR_1}\Bigg)\, e^{(-2\,K_2)iR_1}
\end{aligned}$$

$$\begin{aligned}\therefore P2_2 = {} & P1_1\, e^{(-K_1-K_2)iR_1} + P2_1 e^{(+K_1-K_2)iR_1} \\ & - \frac{1}{2\,V_1K_2}\big(V_1(\,K_2+k)+V_2(K_1-k)\big)P1_1\, e^{(-K_1-K_2)iR_1} \\ & - \frac{1}{2\,V_1K_2}\big(V_1(K_2+k)+\,V_2(-K_1-k)\big)P2_1\, e^{(+K_1-K_2)iR_1}\end{aligned}$$

$$\begin{aligned}\therefore P2_2 = {} & \left(1-\frac{1}{2\,V_1K_2}\big(V_1(\,K_2+k)+V_2(K_1-k)\big)\right)P1_1\, e^{(-K_1-K_2)iR_1} \\ & + \left(1-\frac{1}{2\,V_1K_2}\big(V_1(K_2+k)+\,V_2(-K_1-k)\big)\right)P2_1 e^{(+K_1-K_2)iR_1}\end{aligned}$$

$$\begin{aligned}\therefore P2_2 = {} & \frac{1}{2\,V_1K_2}\Big(2\,V_1K_2-\big(V_1(\,K_2+k)+V_2(K_1-k)\big)\Big)P1_1\, e^{(-K_1-K_2)iR_1} \\ & + \frac{1}{2\,V_1K_2}\Big(2\,V_1K_2-\big(V_1(K_2+k)+\,V_2(-K_1-k)\big)\Big)P2_1 e^{(+K_1-K_2)iR_1}\end{aligned}$$

$$\begin{aligned}\therefore P2_2 = {} & \frac{1}{2\,V_1K_2}\big(2\,V_1K_2-V_1K_2-V_1k-V_2(K_1-k)\big)P1_1\, e^{(-K_1-K_2)iR_1} \\ & + \frac{1}{2\,V_1K_2}\big(2\,V_1K_2-V_1K_2-V_1k-\,V_2(-K_1-k)\big)P2_1 e^{(+K_1-K_2)iR_1}\end{aligned}$$

$$\begin{aligned}\therefore P2_2 = {} & \frac{1}{2\,V_1K_2}\big(\,V_1(K_2-k)-V_2(K_1-k)\big)P1_1\, e^{(-K_1-K_2)iR_1} \\ & + \frac{1}{2\,V_1K_2}\big(\,V_1(K_2-k)-\,V_2(-K_1-k)\big)P2_1 e^{(+K_1-K_2)iR_1}\end{aligned}$$

So then:

$$\begin{aligned}P1_2 = {} & \frac{1}{2\,V_1K_2}\big(V_1(\,K_2+k)+V_2(K_1-k)\big)P1_1\, e^{(-K_1+K_2)iR_1} \\ & + \frac{1}{2\,V_1K_2}\big(V_1(K_2+k)+\,V_2(-K_1-k)\big)P2_1\, e^{(+K_1+K_2)iR_1}\end{aligned} \tag{68}$$

$$\begin{aligned}P2_2 = {} & \frac{1}{2\,V_1K_2}\big(\,V_1(K_2-k)+V_2(-K_1+k)\big)P1_1\, e^{(-K_1-K_2)iR_1} \\ & + \frac{1}{2\,V_1K_2}\big(\,V_1(K_2-k)+\,V_2(+K_1+k)\big)P2_1 e^{(+K_1-K_2)iR_1}\end{aligned} \tag{69}$$

The above is also applicable to the $r = R_2$, with the appropriate change in subscripts. When substituting (59) and (60) we then obtain:

$$\begin{aligned}P1_2 = {} & \frac{1}{2\,V_1K_2}\big(V_1(\,K_2+k)+V_2(K_1-k)\big)\left(\frac{1}{2}-\frac{k\,K_1}{V_1-2k^2}\right)\, e^{(-K_1+K_2)iR_1} \\ & + \frac{1}{2\,V_1K_2}\big(V_1(K_2+k)+\,V_2(-K_1-k)\big)\left(\frac{1}{2}\right. \\ & \left. + \frac{k\,K_1}{V_1-2k^2}\right)\, e^{(K_1+K_2)iR_1}\end{aligned} \tag{70}$$

$$P2_2 = \frac{1}{2\,V_1 K_2}\big(\,V_1(K_2 - k) + V_2(-K_1 + k)\big)\left(\frac{1}{2} - \frac{k\,K_1}{V_1 - 2k^2}\right) e^{(-\,K_1 - K_2)iR_1} + \frac{1}{2\,V_1 K_2}\big(\,V_1(K_2 - k) + V_2(+K_1 + k)\big)\left(\frac{1}{2} + \frac{k\,K_1}{V_1 - 2k^2}\right) e^{(K_1 - K_2)iR_1} \tag{71}$$

3.4.4 Region Three: $R_2 < r < \infty$

We then have the following:

$$P1 = P1_3$$

$$P2 = P2_3$$

$$V = V_3 = 0$$

$$K = K_3 = \sqrt{k^2} = k$$

$$F_{03}^{(in)}(E,r) = P1_3\, e^{(k-\,k)ir} + P2_3 e^{(k+\,k)ir} = P1_3 + P2_3 e^{2kir} \tag{72}$$

$$\begin{aligned} F_{03}^{(out)}(E,r) &= \left(1 - \frac{2k^2}{V_2} + \frac{2k}{V_2}k\right) P1_3\, e^{(-k-\,k)ir} \\ &\quad + \left(1 - \frac{2k^2}{V_2} - \frac{2k}{V_2}k\right) P2_3\, e^{(-k+\,k)ir} \\ &= P1_3\, e^{-2kir} + \left(1 - \frac{4k^2}{V_2}\right) P2_3 \end{aligned} \tag{73}$$

We know that the following holds, since it was calculated for the preceding region:

$$P1_3 = \frac{1}{2\,V_2 K_3}\big(V_2(\,K_3 + k) + V_3(K_2 - k)\big) P1_2\, e^{(-\,K_2 +\,K_3)iR_2} + \frac{1}{2\,V_2 K_3}\big(V_2(K_3 + k) + V_3(-K_2 - k)\big) P2_2\, e^{(+\,K_2 +\,K_3)iR_2}$$

$$P2_3 = \frac{1}{2\,V_2 K_3}\big(\,V_2(K_3 - k) + V_3(-K_2 + k)\big) P1_2\, e^{(-\,K_2 - K_3)iR_2} + \frac{1}{2\,V_2 K_3}\big(\,V_2(K_3 - k) + V_3(+K_2 + k)\big) P2_2 e^{(+\,K_2 - K_3)iR_2}$$

When substituting $V_3 = 0$ and $K_3 = k$, we then obtain:

$$P1_3 = \frac{1}{2V_2 k}\big(V_2(\,k + k)\big) P1_2\, e^{(-\,K_2 +\,k)iR_2} + \frac{1}{2V_2 k}\big(V_2(k + k)\big) P2_2\, e^{(+\,K_2 +\,k)iR_2}$$

$$\therefore P1_3 = P1_2\, e^{(-\,K_2 +\,k)iR_2} + P2_2\, e^{(+\,K_2 +\,k)iR_2}$$

And also:

$$P2_2 = \frac{1}{2V_2k}(\,0+0)P1_2\,e^{(-\,K_2-K_3)iR_2} + \frac{1}{2V_2k}(\,0+\,0)P2_2e^{(+\,K_2-K_3)iR_2}$$

$$\therefore P2_3 = 0$$

So:

$$\therefore P1_3 = P1_2\,e^{(-\,K_2+\,k)iR_2} + P2_2\,e^{(+\,K_2+\,k)iR_2} \tag{74}$$

$$P2_3 = 0 \tag{75}$$

This means that (72)and (73) becomes:

$$\begin{aligned} F_{03}^{(in)}(E,r) &= \left(P1_2\,e^{(-\,K_2+\,k)iR_2} + P2_2\,e^{(+\,K_2+\,k)iR_2}\right)e^{(k-\,k)ir} + (0)e^{(k+\,k)ir} \\ &= P1_2\,e^{(-\,K_2+\,k)iR_2} + P2_2\,e^{(+\,K_2+\,k)iR_2} \end{aligned}$$

$$\begin{aligned} F_{03}^{(out)}(E,r) &= \left(P1_2\,e^{(-\,K_2+\,k)iR_2} + P2_2\,e^{(+\,K_2+\,k)iR_2}\right)e^{-2kir} + \left(1-\frac{4k^2}{V_2}\right)(0) \\ &= P1_2\,e^{(-\,K_2+\,k)iR_2-2kir} + P2_2\,e^{(+\,K_2+\,k)iR_2-2kir} \end{aligned}$$

Thus:

$$F_{03}^{(in)}(E,r) = P1_2\,e^{(-\,K_2+\,k)iR_2} + P2_2\,e^{(+\,K_2+\,k)iR_2} \tag{76}$$

$$F_{03}^{(out)}(E,r) = P1_2\,e^{(-\,K_2+\,k)iR_2-2kir} + P2_2\,e^{(+\,K_2+\,k)iR_2-2kir} \tag{77}$$

With $P1_2$ and $P2_2$ given by equations (70) and (71).

3.4.5 The Jost Equations

From (28) and (29), the Jost functions are given by:

$$f_l^{(in)}(E) = \lim_{r\to\infty} F_l^{(in)}(E,r)$$

$$f_l^{(out)}(E) = \lim_{r\to\infty} F_l^{(out)}(E,r)$$

For our specific potential:

$$f_l^{(in)}(E) = \lim_{r\to\infty} F_l^{(in)}(E,r) = \lim_{r\to R_2} F_0^{(in)}(E,r) = F_{03}^{(in)}(E,R_2)$$

$$f_l^{(out)}(E) = \lim_{r\to\infty} F_l^{(out)}(E,r) = \lim_{r\to R_2} F_0^{(out)}(E,r) = F_{03}^{(out)}(E,R_2)$$

Thus, when substituting (76) and (77):

$$f_0^{(in)}(E) = P1_2\,e^{(-\,K_2+\,k)iR_2} + P2_2\,e^{(+\,K_2+\,k)iR_2} \tag{78}$$

$$f_0^{(out)}(E) = P1_2\,e^{(-\,K_2-\,k)iR_2} + P2_2\,e^{(+\,K_2-k)iR_2} \tag{79}$$

With $P1_2$ and $P2_2$ given by equations (70) and (71).

Finally we have the Jost equations!

4. Results

4.1 Concerning Units

I provide a short explanation pertaining to the units of the variables used in this paper. We have the following, by definition, from equation (13):

$$k^2 = \frac{2\mu E}{\hbar^2}$$

The unit of a symbol will be indicated by placing the symbol in square brackets. So, we have the following:

$$[k]^2 = \frac{[\mu][E]}{[\hbar]^2}$$

Energy can be given in MeV and mass in MeV/c^2, with c the speed of light in a vacuum. Thus:

$$[k]^2 = \frac{(MeVc^2/)(MeV)}{[\hbar]^2}$$

$$\therefore [k]^2 = \frac{(MeV)^2}{[c]^2[\hbar]^2}$$

$$\therefore [k] = \frac{(MeV)}{[c\hbar]}$$

We can write the factor $c\hbar$ as 197 $MeV\ fm$. Thus $[c\hbar] = MeV\ fm$:

$$\therefore [k] = \frac{(MeV)}{MeV\ fm}$$

$$\therefore [k] = \frac{1}{fm}$$

Thus k will be given in inverse femto-meter, fm^{-1}. It follows that r is given in fm. Also, mass will be given simply in MeV, since it is obvious that the c is unnecessary if, in stead of $c\hbar$, we let:

$$\hbar = 197\ MeV\ fm \qquad (80)$$

To sum up, then: Energy and potential are given in MeV, since they are related. Mass, and equivalent mass, are also given in MeV. k is given in fm^{-1}, and r in fm. In choosing these units, the data becomes significantly more manageable. Most papers that make use of Quantum Mechanics do not explain the use of specific units, which can lead to much confusion. This is why I include this bit of dimensional analysis.

4.2 The Spectral Points

The search for the spectral points is a tiresome affair, since the expression for $f_0^{(in)}(E)$ is far from simple. Thus it must be numerically solved using some form of mathematical programming software. I make use of *Maple*, and the coding I used is enclosed as Appendix A.

A huge problem I encountered in searching for spectral points is that generally the program gives only one value, and stops the search, unless it is told to ignore the found value and proceed. The values that are obtained in such a manner are haphazard and unreliable, since some of the bound states appear to be missing.

Thankfully, I was able to find a method that works admirably: if the search is conducted close to a specific real value, and further searches are conducted at real values at small discreet steps from the previous value, the chances of obtaining all the bound states increase dramatically. Since there are infinitely many resonant states, it is sufficient to find a relatively small number of them to be able to make reliable conclusions.

The only flaw in this method is that very large bound state values will typically not be found, since the search is conducted at a starting point of -1 and ends at 1. Values much larger than 1 are found, which is encouraging, but there is no guarantee that all large bound states are located. Even so, the results look promising.

The values chosen for the radii and the potential magnitudes of the step-potential, as well as the equivalent mass, are chosen in such a way to correspond roughly to actual experimental data. For example, the mass of a proton is slightly larger than $900\,Mev$ and that of an electron is roughly $0.5\,Mev$. Thus equivalent masses in this range, as well as significantly larger values, are researched. The same applies to the other choices.

We want to research the effect a change in any of these values has on the spectral points. This cannot be done all at once, thus the effect of each is considered separately.

4.2.1 Change in Equivalent Mass, μ

The following standard values for the other variables are chosen:

$R_1 = 7.5\,fm$
$R_2 = 15\,fm$
$U_1 = -100\,MeV$
$U_1 = 100\,MeV$

The data obtained is graphically represented in the k-plane. Note that, if not clearly indicated, μ is given in MeV, R in fm, and either U in MeV.

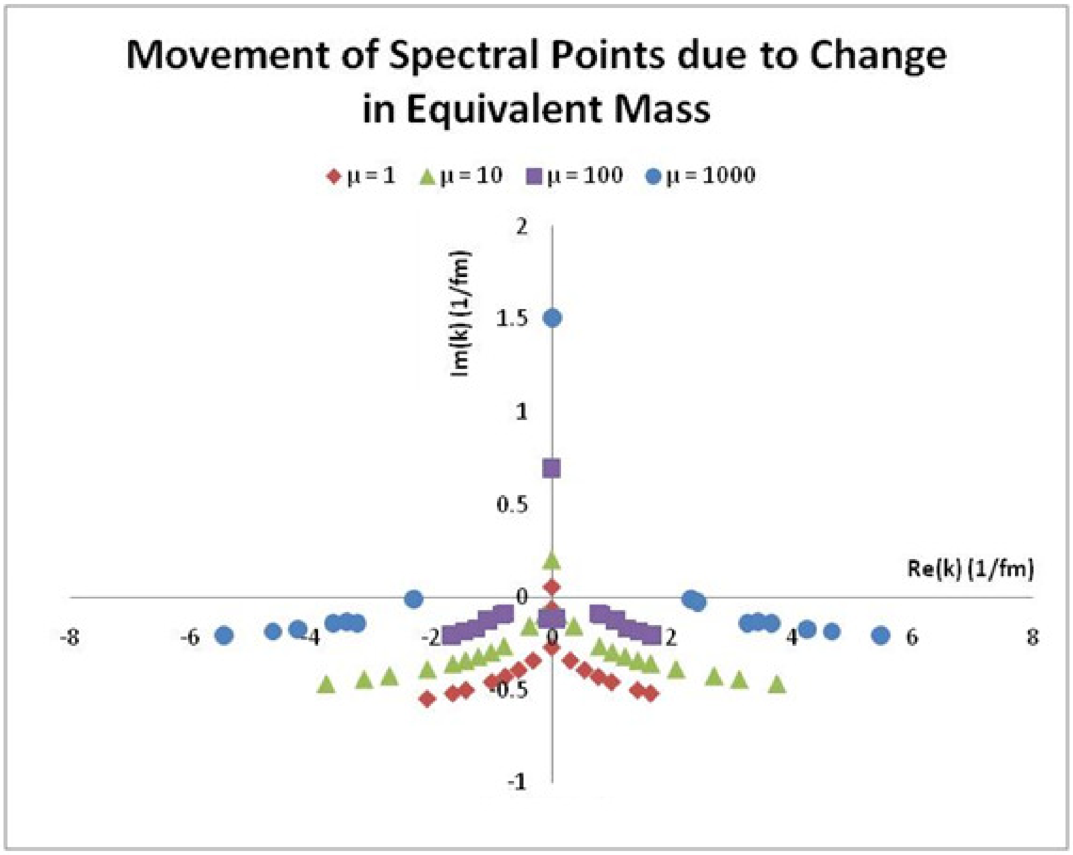


Figure 4

It is wonderfully clear that the bound state energies become larger as μ becomes larger. Also, the imaginary part of the resonance zeros move significantly closer zero for greater μ. This indicates that the resonance energies are small, and that they are of small width. It is also interesting to note that the virtual states occur for small μ only; specifically $\mu = 1$.

4.2.2 Change in Radii, R_1 and R_2

The following standard values for the other variables are chosen:

$\mu = 100 MeV$
$U_1 = -100\ MeV$
$U_2 = 100\ MeV$

Let us first consider a scenario where $R_2 - R_1$ is much larger than R_1:

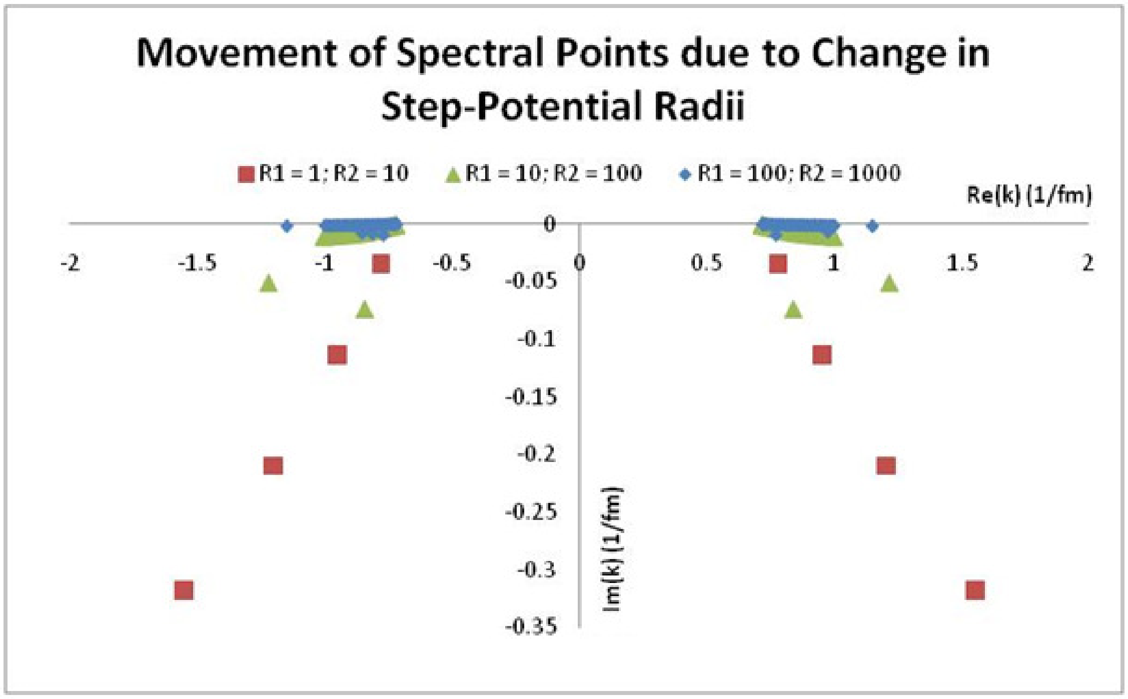


Figure 5

Clearly, there are no bound or virtual states. Note also that $R_2 = 10R_1$ in all three plots in Figure 3, and that the greater either R is, the closer $Im(k)$ is to zero. As was the case with an increase in μ, this is indicative of small resonance energies that have small width, and thus have large half-lives. Although the data is not given here, where $R_2 = 100R_1$ and $R_2 = 1000R_1$, similar plots are obtained.

Let us now consider a scenario where $R_2 - R_1$ is much smaller than R_1:

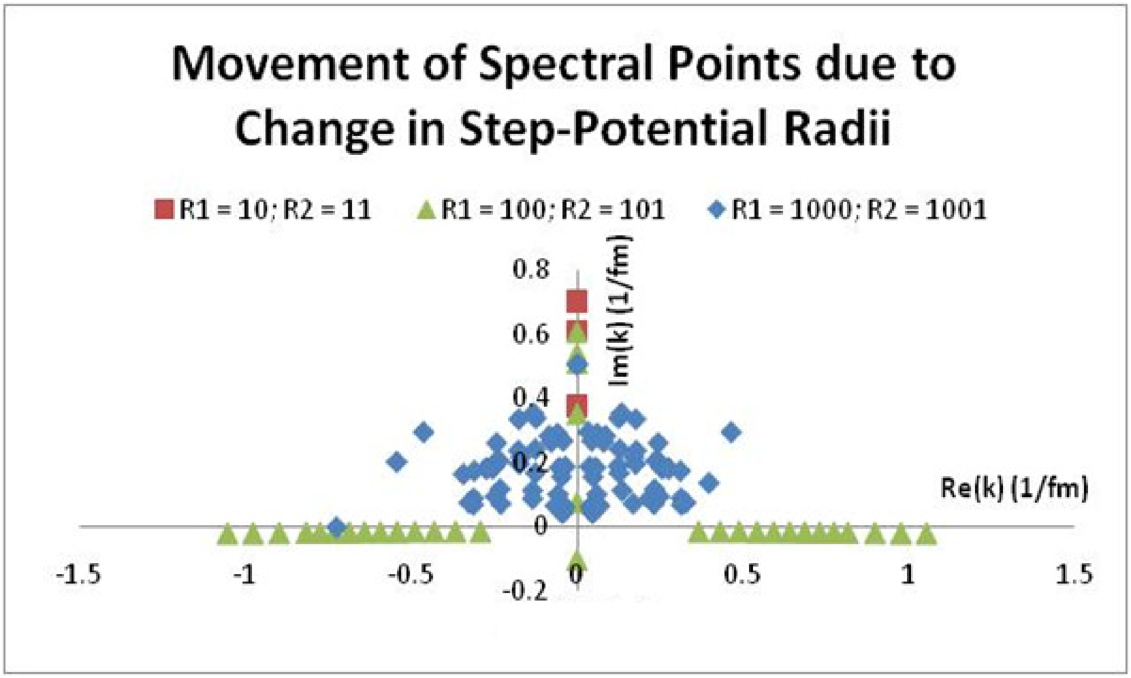


Figure 6

Table 1: Table indicating the number of bound states for the systems of Figure 5

	$R_1 = 10;\ R_2 = 11$	$R_1 = 100;\ R_2 = 101$	$R_1 = 1000;\ R_2 = 1001$
Im(k) values			
	0.706672885	0.510263108	0.50606993
	0.375796676	0.538687025	0.509200897
	0.611580467	0.075237767	-
	-	0.351360465	-
	-	0.607189389	-
Number of Bound States	3	5	2

It appears that, unlike Figure 4, there is an abundance of bound states if $R_2 - R_1$ is much smaller than R_1. Yet these bound states do not decrease or increase with greater values of either R. It may be that all the bound states of the systems have not been found, and if this is the case, better conclusions may be drawn with better data.

It would be foolish to assume that there are no resonance states for the system where $R_1 = 10$ and $R_2 = 11$, since there can be infinitely many. The program for finding the spectral points concentrates its search in an area relatively close to zero, thus it would seem that the resonances for this system are at much larger values.

On the other hand, the system where $R_1 = 1000$ and $R_2 = 1001$ has an abundance of complex roots in the area under consideration. Most of these roots are not even shown in Figure 4, since the plot then becomes confusing. Not all these complex roots represent resonant states, but a sufficiently vast number certainly do: we can thus conclude that sufficiently large values of R_1 with small R_2 result in a system with an incredibly large concentration of resonance states. To justify this statement, consider the following:

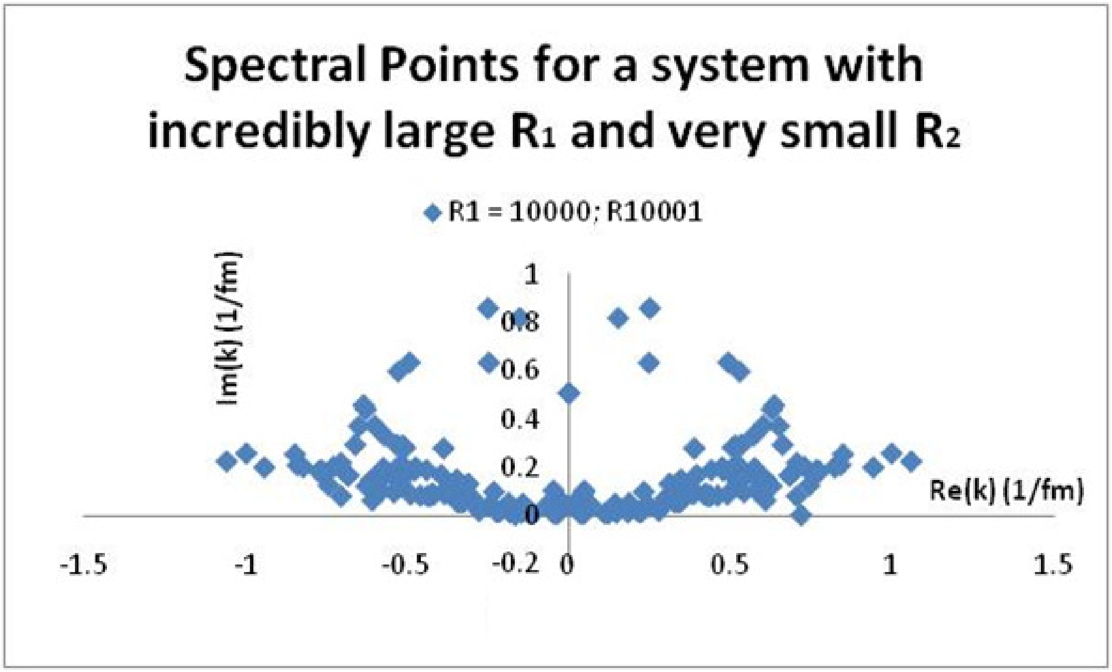


Figure 7

Note that there are only two bound states at:

$Im(k) = 0.507525\ 1/fm$ and $Im(k) = 0.508153\ 1/fm$

This is not clear from the plot due to the over-abundance of points.

We will finally consider a situation where R_1 and $R_2 - R_1$ are exactly the same:

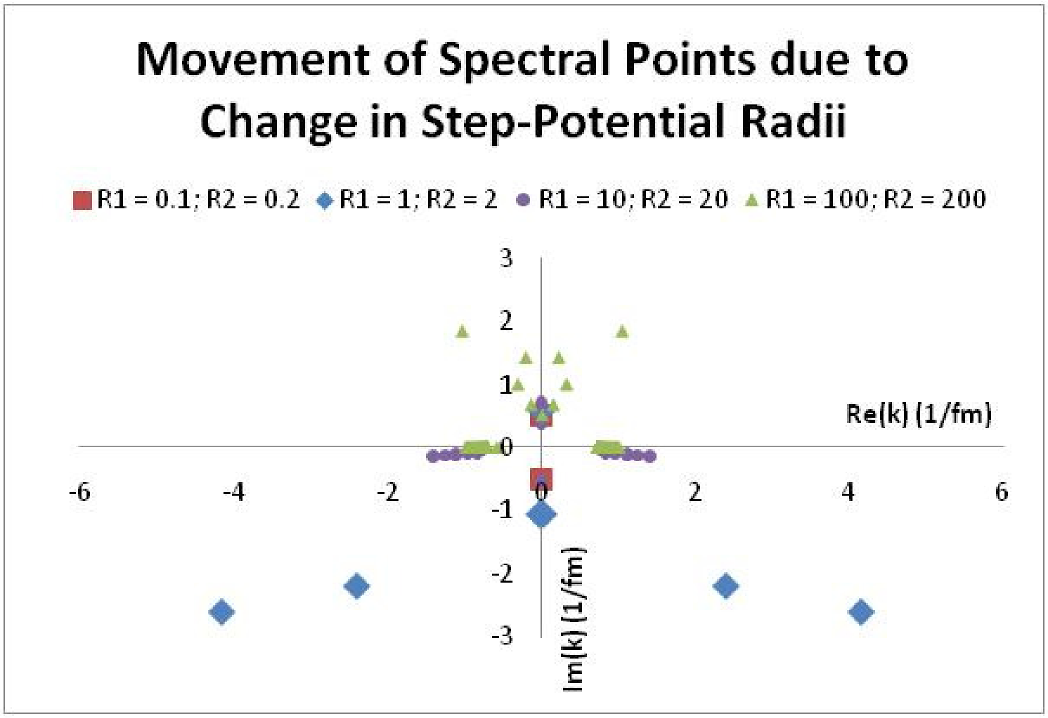


Figure 8

All the systems have bound states, but nothing conclusive can be said about the number or position of said states. The resonances, on the other hand, seem to decrease as the radii increase.

4.2.3 Change in Potentials, U_1 and U_1

The following standard values for the other variables are chosen:

$\mu = 100MeV$
$R_1 = 7.5\ fm$
$R_2 = 15\ fm$

Firstly, we consider spectral points for systems where U_1 is held constant at -1 MeV throughout, and U_2 varies:

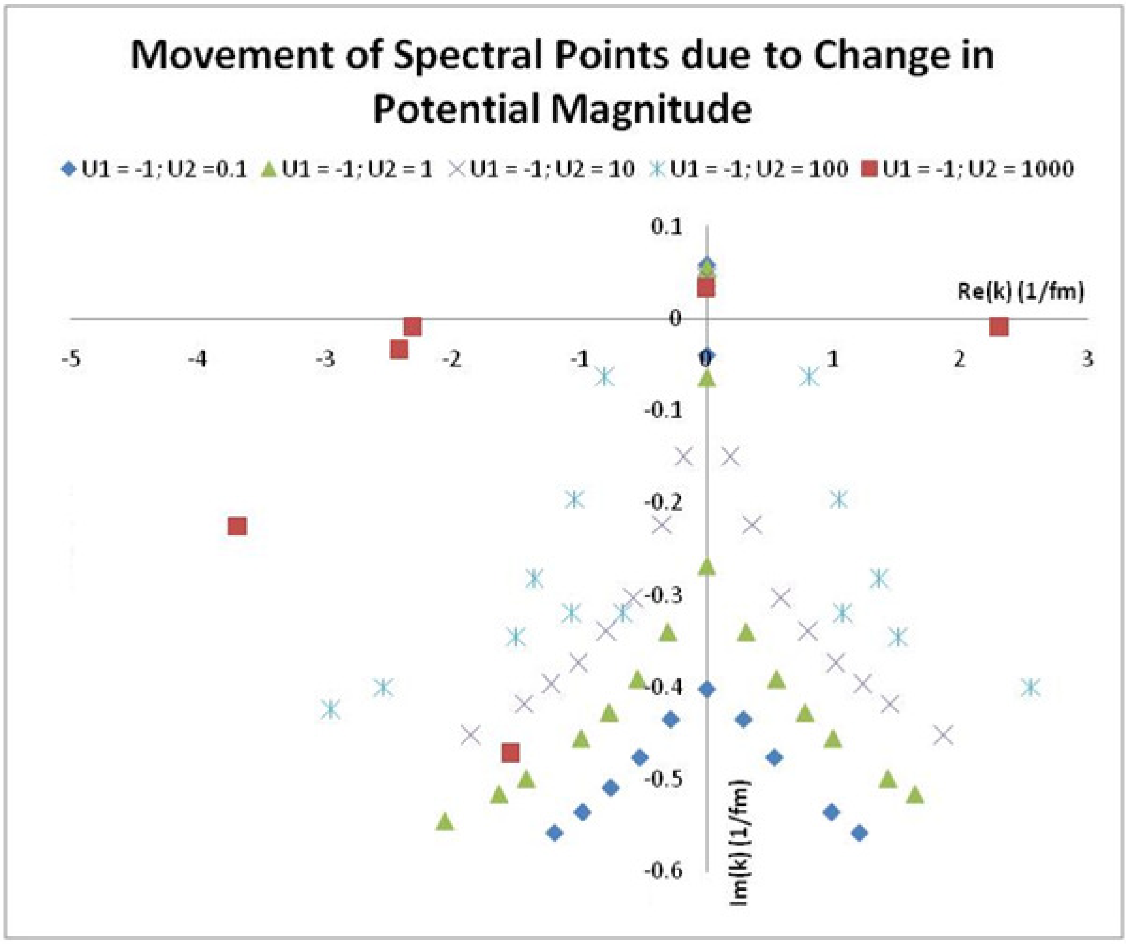


Figure 9

From Figure 9 it is clear that resonances move further away from the $Re(k)$ axis as the second potential increases. Also, virtual states are present for the two small values of U_2.

Figure 10 contains the same data as Figure 9, but shows only the bound states:

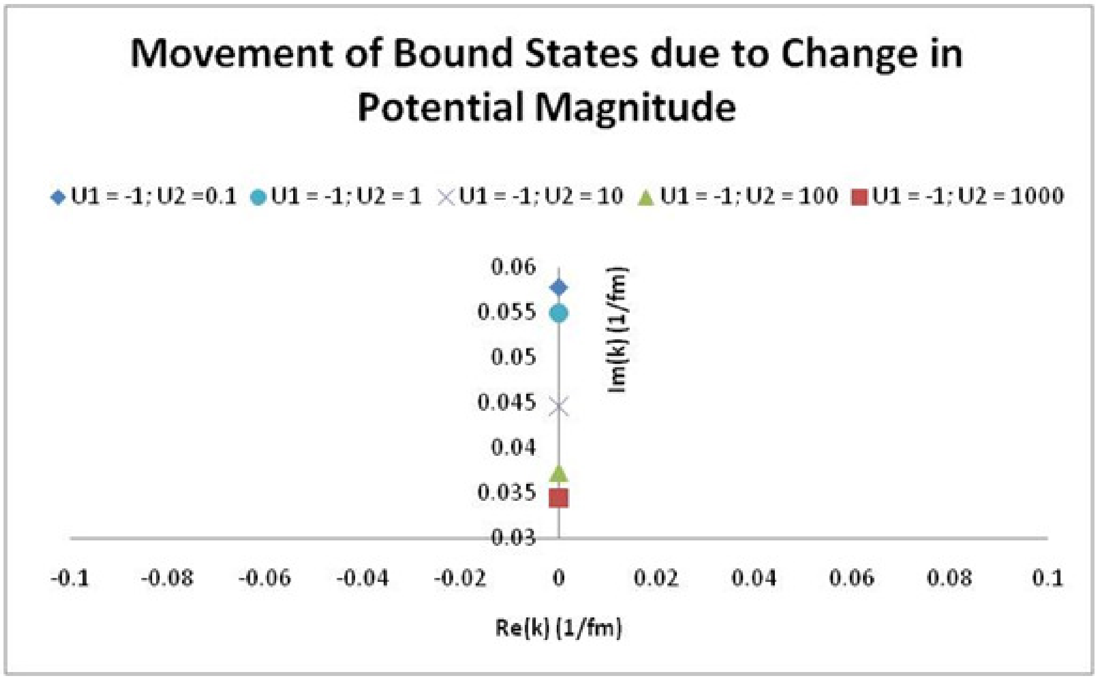


Figure 10

From Figure 10 it is clearer that each system has only one bound state, and that the magnitude of the energy of this state increases as the U_2 increases.

Now, we consider spectral points for systems where U_2 is held constant at $1\,MeV$ throughout, and U_1 varies. I draw two graphs; one of the resonant states, and one of the bound and virtual states:

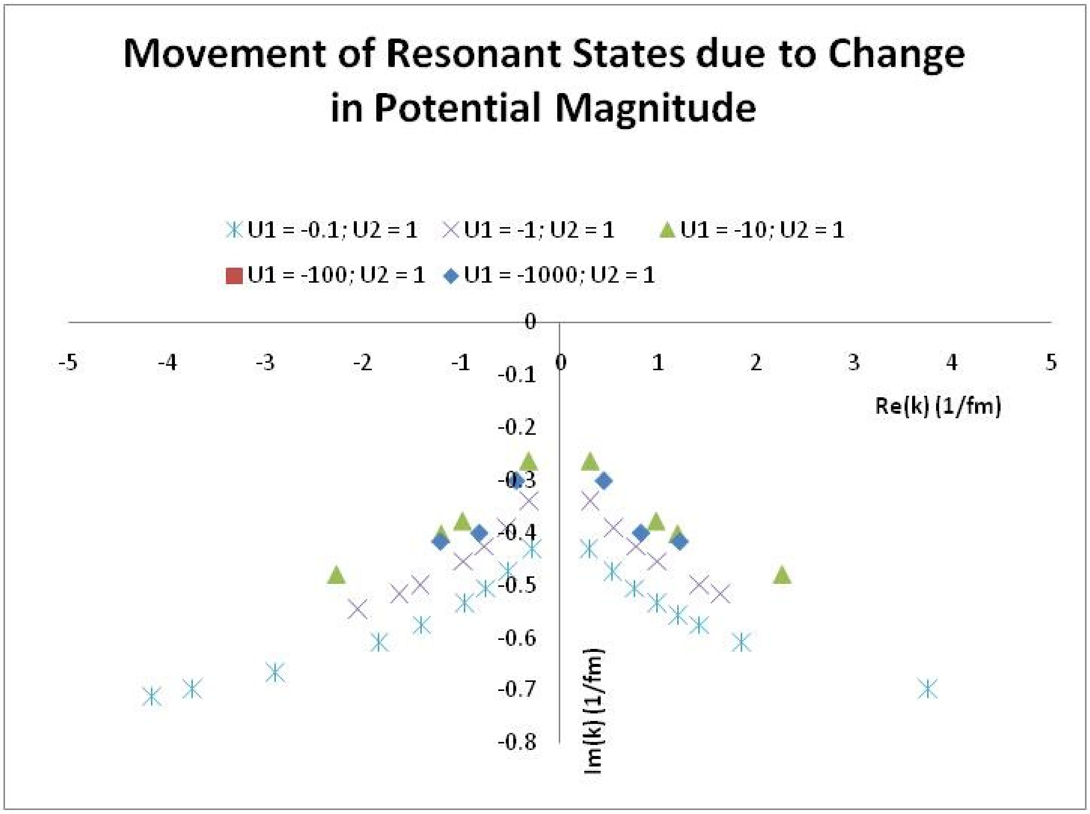

Movement of Resonant States due to Change in Potential Magnitude
U1 = -0.1; U2 = 1
U1 = -1; U2 = 1
U1 = -10; U2 = 1
U1 = -100; U2 = 1
U1 = -1000; U2 = 1
0
-5
-4
-3
-2
-1
0
1
2
3
4
5
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
-0.7
-0.8
Re(k) (1/fm)
Im(k) (1/fm)

Figure 11

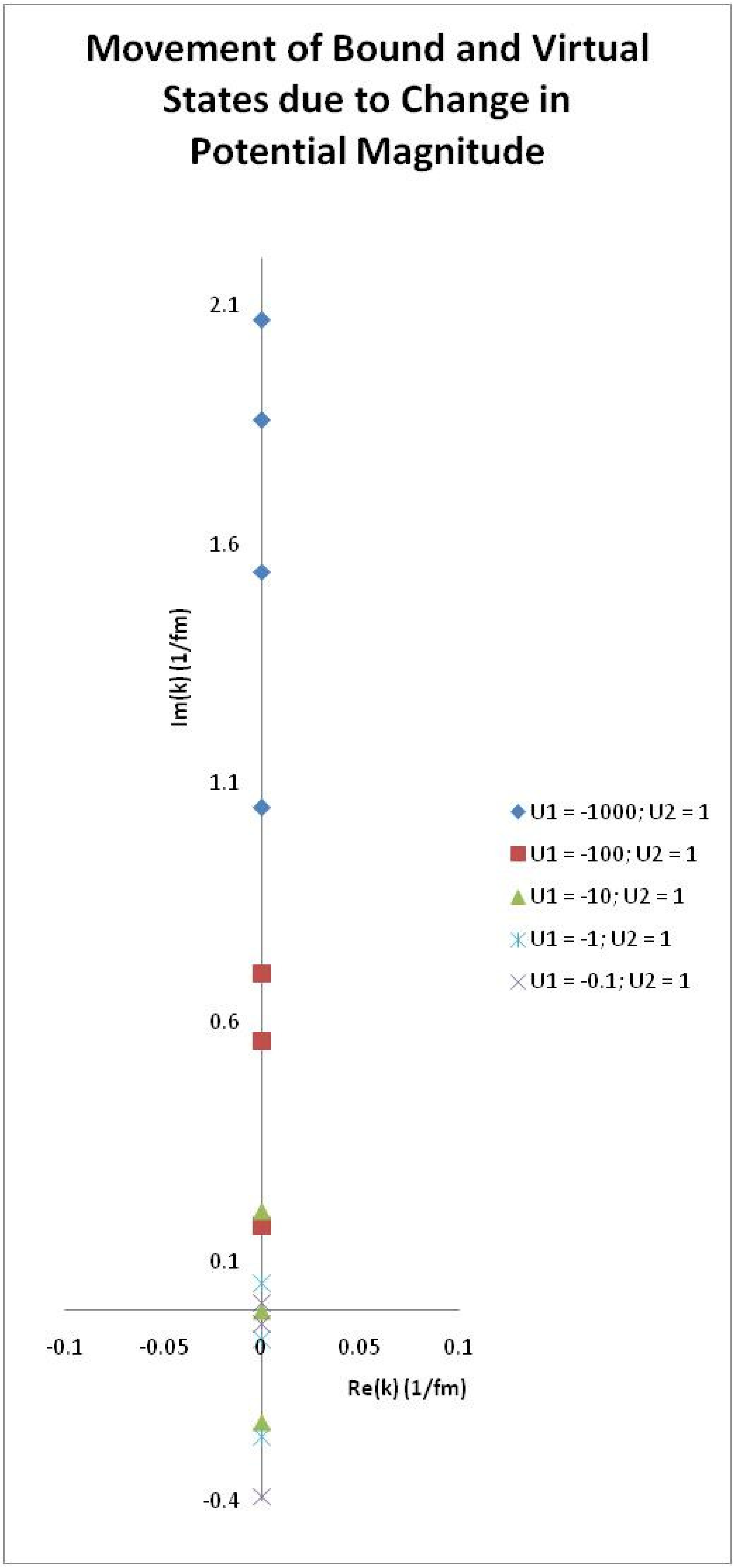

Movement of Bound and Virtual States due to Change in Potential Magnitude
2.1
1.6
1.1
0.6
0.1
-0.4
Im(k) (1/fm)
-0.1
-0.05
0
0.05
0.1
Re(k) (1/fm)
◆ U1 = -1000; U2 = 1
■ U1 = -100; U2 = 1
▲ U1 = -10; U2 = 1
✳ U1 = -1; U2 = 1
× U1 = -0.1; U2 = 1

Figure 12

It is interesting that there does not seem to be a relationship between U_1 and the resonant states, as was the case with varying U_2. Once again, though, there are more virtual states for smaller U_1 and a definite increase in bound states for greater U_1. The states seem to shift upwards along the $Im(k)$ axis.

Finally we consider systems where the U_1 is equal to U_2, but with opposite sign. Again, two graphs are drawn:

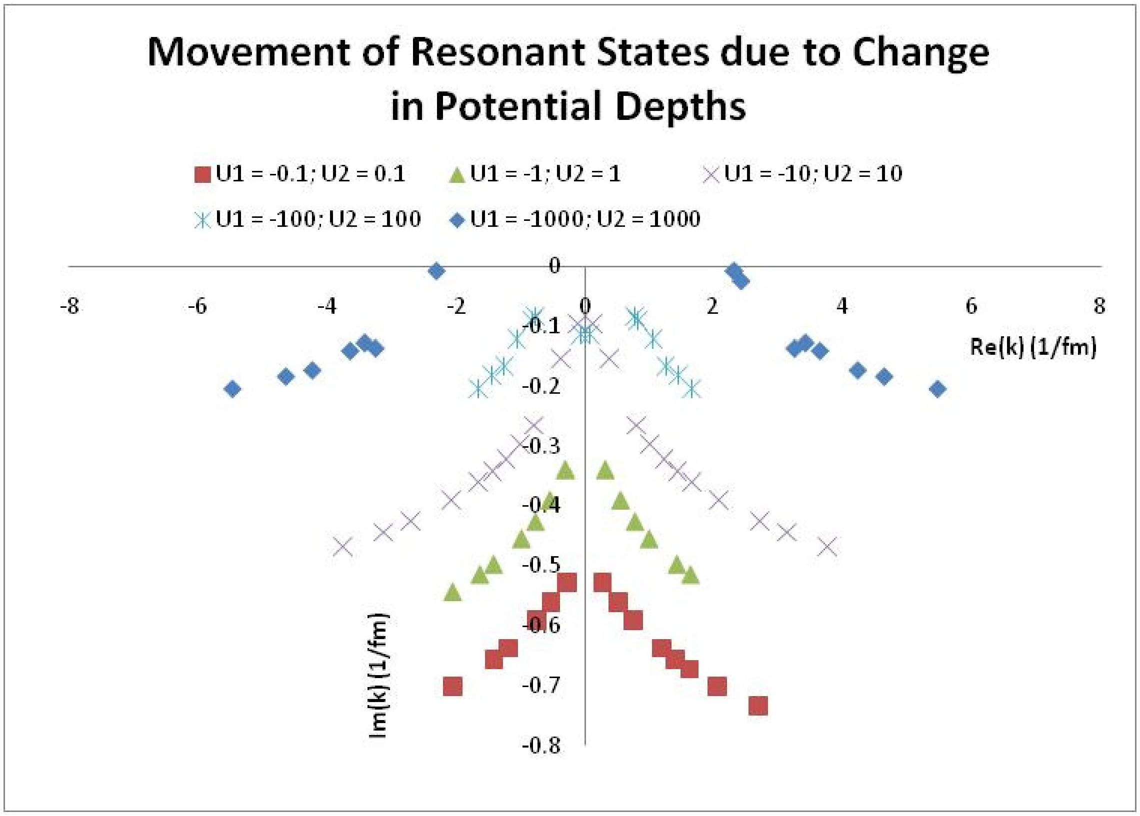

Movement of Resonant States due to Change in Potential Depths
U1 = -0.1; U2 = 0.1
U1 = -1; U2 = 1
U1 = -10; U2 = 10
U1 = -100; U2 = 100
U1 = -1000; U2 = 1000
Re(k) (1/fm)
Im(k) (1/fm)
-8
-6
-4
-2
0
2
4
6
8
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
-0.7
-0.8

Figure 13

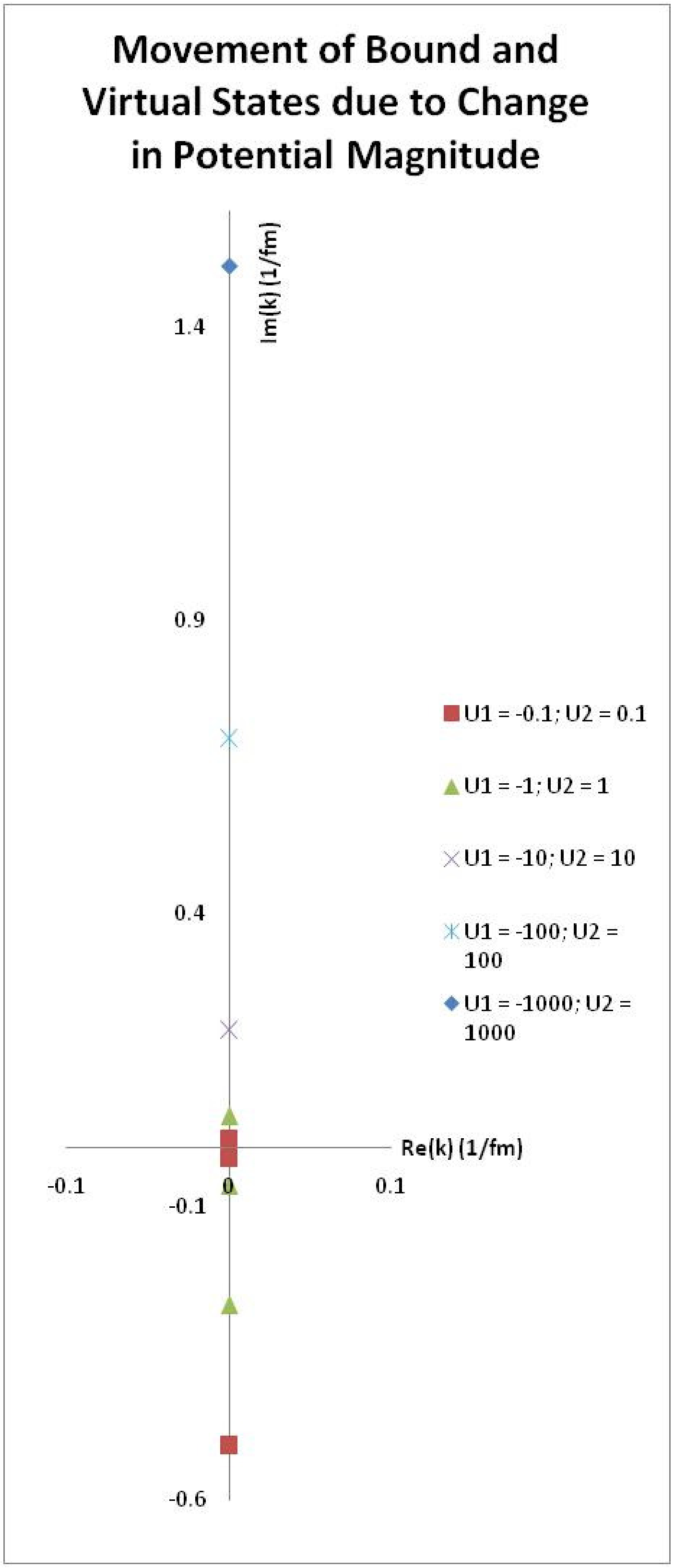

Movement of Bound and Virtual States due to Change in Potential Magnitude
Im(k) (1/fm)
1.4
0.9
0.4
-0.1
-0.6
Re(k) (1/fm)
-0.1
0
0.1
U1 = -0.1; U2 = 0.1
U1 = -1; U2 = 1
U1 = -10; U2 = 10
U1 = -100; U2 = 100
U1 = -1000; U2 = 1000

Figure 14

Here we have a general increase in potential depth. Resonant state energies are small and have smaller width as the depths increase, there are more virtual states for small potential depths, but, interestingly, there is no increase in bound states with an increase in potential depth. This is provided that all the bound states have been found, which is not necessarily the case. Yet even the medium sized potentials have only one bound state, where in other scenarios there were more. We will thus assume that all bound states are found, and that there is no increase in bound states for a general increase in potential depth.

5. Conclusions

Firstly, we can most certainly conclude that the state of the system is dependent on the equivalent mass of the system, radially dependant, and dependant on the depth of the potential.

A system with small equivalent mass will have more virtual states, and less bound states. For a system with greater mass, the virtual states become bound states: there is sufficient energy. In fact, as the mass increases, the bound state energy increases. An increase in mass will therefore cause in increase in energy.

Also, the placement of the complex roots indicate a definite decrease in resonant state energies and an increase in "lifespan" of these energies. Particles in a system with a large equivalent mass will thus most likely be in the bound state, or in a state that is practically bound.

For a system with a small first radius and a large second radius, where the negative potential is in other words very sharp, no bound or virtual states are evident, and the resonances again decrease in size and width, as the radii become larger. This is understandable if we take the negative potential to be attractive and the positive potential to be repulsive: the repulsive potential overpowers the attractive potential since it exists in a much larger area.

When we consider a system where the first radius is significantly larger than the second, there is an abundance of bound states. In this case, the attractive potential covers a larger area than the repulsive potential; thus more bound states can, in fact, be expected. It is a pity that it cannot be said that the number of bound states increase proportionately with an increase in the first radius. Further study will have to be done to ascertain if there is a relationship. The data obtained concerning the resonant and virtual states in this system is also unsatisfactory, since no logical conclusion can be drawn from it.

When we look at large differences between the potentials, the hypothesis that the size of- and area covered by the attractive and repulsive potentials directly influences the bound states is, thankfully, justified:

For a small negative potential and a large positive potential, there is no decrease in bound states, but there is no increase in bound states either: in all systems we calculated, there is only one bound state. Also, there is a marked increase in bound states as the negative potential is increased sufficiently to overpower the positive potential, where the attraction is greater than the repulsion, in other words.

Once again, there is little we can say about the resonance states. They certainly move up and out as either potential increases, but since there appears to be equal change in $Im(k)$ and $Re(k)$, the values of $Im(E)$ and $Re(E)$ will stay roughly the same as the potential increases.

Finally, for the systems where both radii and both potentials are the same, we can draw three conclusions: firstly, the data does not contradict our previous conclusion. Secondly, we can clearly see that there are no virtual states for smaller potentials and greater potentials result in bound states of larger energies. Thirdly, it seems that larger radii as well as larger potentials result in smaller resonances of greater lifespan.

6. Discussion

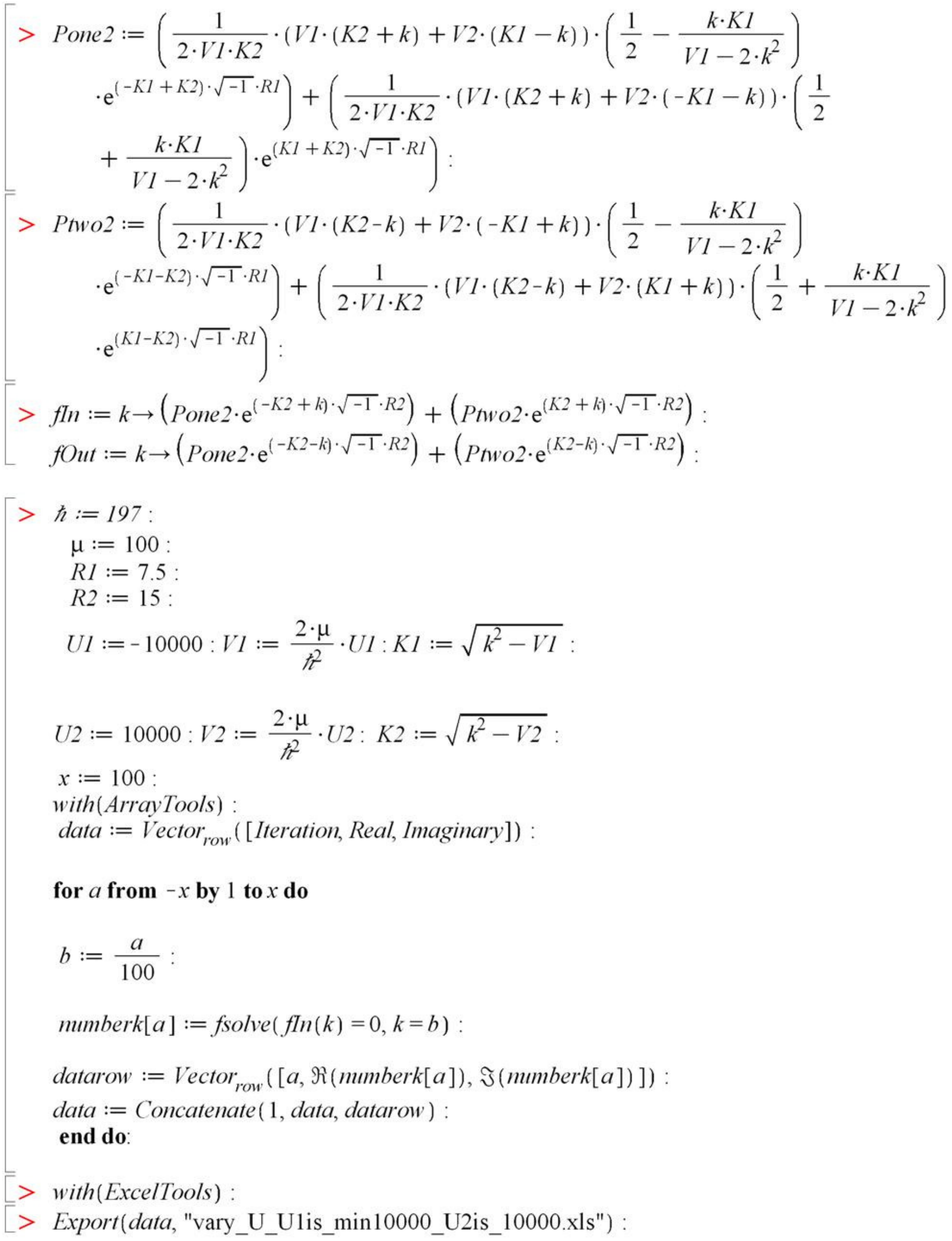
One may now ask what the point was of all that trouble to make these few rather obvious conclusions. It seems hardly worth the effort, yet there are two highly valuable reasons:

The fact that the conclusions coincide perfectly with what is generally expected is very encouraging: it is a reliable indication that the theory works. The simple fact that the data behaves in a way that it is expected to behave, should not be sneered at; it is a remarkable feat. It enables us to apply this theory to physical potentials with the greatest of confidence, to obtain much needed data on quantum systems to predict information on scattering, as well as justifying experimental data.

Also, after months of misunderstandings, dead ends, faulty programming, misinterpretation of data, and stress in general, I can safely say that I have a very good understanding of the basics of Jost Functions and their application to scattering problems.

7. Appendix A

An example of the code used :



$$> \mathit{Pone2} := \left(\frac{1}{2\cdot V1\cdot K2}\cdot\left(V1\cdot(K2+k)+V2\cdot(K1-k)\right)\cdot\left(\frac{1}{2}-\frac{k\cdot K1}{V1-2\cdot k^2}\right)\cdot e^{(-K1+K2)\cdot\sqrt{-1}\cdot R1}\right)+\left(\frac{1}{2\cdot V1\cdot K2}\cdot\left(V1\cdot(K2+k)+V2\cdot(-K1-k)\right)\cdot\left(\frac{1}{2}+\frac{k\cdot K1}{V1-2\cdot k^2}\right)\cdot e^{(K1+K2)\cdot\sqrt{-1}\cdot R1}\right):$$

$$> \mathit{Ptwo2} := \left(\frac{1}{2\cdot V1\cdot K2}\cdot\left(V1\cdot(K2-k)+V2\cdot(-K1+k)\right)\cdot\left(\frac{1}{2}-\frac{k\cdot K1}{V1-2\cdot k^2}\right)\cdot e^{(-K1-K2)\cdot\sqrt{-1}\cdot R1}\right)+\left(\frac{1}{2\cdot V1\cdot K2}\cdot\left(V1\cdot(K2-k)+V2\cdot(K1+k)\right)\cdot\left(\frac{1}{2}+\frac{k\cdot K1}{V1-2\cdot k^2}\right)\cdot e^{(K1-K2)\cdot\sqrt{-1}\cdot R1}\right):$$

$$> \mathit{fIn} := k\rightarrow\left(\mathit{Pone2}\cdot e^{(-K2+k)\cdot\sqrt{-1}\cdot R2}\right)+\left(\mathit{Ptwo2}\cdot e^{(K2+k)\cdot\sqrt{-1}\cdot R2}\right):$$

$$\mathit{fOut} := k\rightarrow\left(\mathit{Pone2}\cdot e^{(-K2-k)\cdot\sqrt{-1}\cdot R2}\right)+\left(\mathit{Ptwo2}\cdot e^{(K2-k)\cdot\sqrt{-1}\cdot R2}\right):$$

$> \hbar := 197:$

$\mu := 100:$

$R1 := 7.5:$

$R2 := 15:$

$$U1 := -10000 : V1 := \frac{2\cdot\mu}{\hbar^2}\cdot U1 : K1 := \sqrt{k^2-V1}:$$

$$U2 := 10000 : V2 := \frac{2\cdot\mu}{\hbar^2}\cdot U2 : K2 := \sqrt{k^2-V2}:$$

$x := 100:$

with(*ArrayTools*) :

$\mathit{data} := \mathit{Vector}_{\mathit{row}}([\mathit{Iteration}, \mathit{Real}, \mathit{Imaginary}]):$

for *a* **from** $-x$ **by** 1 **to** *x* **do**

$$b := \frac{a}{100}:$$

$\mathit{numberk}[a] := \mathit{fsolve}(\mathit{fIn}(k)=0, k=b):$

$\mathit{datarow} := \mathit{Vector}_{\mathit{row}}([a, \Re(\mathit{numberk}[a]), \Im(\mathit{numberk}[a])]):$

$\mathit{data} := \mathit{Concatenate}(1, \mathit{data}, \mathit{datarow}):$

end do:

> *with*(*ExcelTools*) :

> *Export*(*data*, "vary_U_U1is_min10000_U2is_10000.xls") :

8. References

[1] S. A. Rakityansky, *Jost functions in Quantum Mechanics: Theory and Guide to Applications* (University of South Africa, Pretoria)

[2] S. A. Rakityansky, S. A. Sofianos, K. Amos, *A Method of Calculating the Jost Function for Analytic Potentials* (University of South Africa, 1995)

[3] *Lecture Notes: Jost functions in Quantum Mechanics,* Compiled by S. A. Rakityansky (University of South Africa, Pretoria, 2007)

[4] *Lecture Notes: PHY703 Quantum Mechanics Lectures 1-15,* Compiled by S. A. Rakityanski (University of Pretoria, 2010)

[5] N. Zettili, *Quantum Mechanics* (John Wiley & Sons, Ltd., 3rd edition, New York, 2001)

[6] J. R. Taylor, C. D. Zafiratos, M. A. Dubson, *Modern Physics for Scientists and Engineers*, (Prentice Hall, Inc.,2nd edition, New Jersey, 2004)

[7] K. F. Riley, M. P. Hobson, S. J. Bence, *Mathematical Methods for Physics and Engineering,* (Cambridge University Press, 1998)

[8] J. S. De Villiers, *Interaction of the Eta-Meson with Light Nuclei*, (University of South Africa, 2005)