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Bachelor Project Mathematics and Physics

# Quantum Monodromy and Complex Scaling

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**Abstract.** In this thesis, we will consider classical and quantum monodromy in the champagne bottle potential. After a review of the necessary techniques from quantum mechanics, we study how action-angle variables lead to monodromy in the champagne bottle. Moreover, we will numerically determine the spectrum of this potential, and observe that there is quantum monodromy in the system. Finally, we will determine the resonance spectrum of the upside-down champagne bottle to see if there is also monodromy here. Conclusive evidence for this was not found.

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# Introduction

The Wikipedia definition of monodromy is the study of how mathematical objects behave when they run around a singularity. In their article, they give the example of the complex logarithm, which increases by $2\pi$ as we move around the unit circle. A consequence of this fact, is that it is impossible to define a single-valued logarithm on the whole complex plane.

Similar phenomena occur in classical and quantum mechanical systems. Monodromy was first studied in classical mechanics by Duistermaat [8]. According to the Arnold-Liouville theorem, we can study the local structure of integrable systems, which will be defined in Chapter 2, in terms of action-angle variables [2]. Duistermaat studies the global properties of these variables. It turns out that there are many systems in which it is not possible to define global action-angle variables, due to a topological obstruction. Examples of these systems include the spherical pendulum [10], and the champagne bottle [4], [6].

A similar phenomenon happens in the quantum mechanical equivalents of these systems. This was first discovered by Cushman and Duistermaat in the spherical pendulum [7]. Since then, quantum monodromy has been studied intensively.

In this thesis, we are interested in studying monodromy in scattering problems. When a potential is turned upside down, we can find the resonance spectrum of the system by complex scaling, which we will study in Chapter 3. It can be shown that the spectrum of a potential which supports bound states is related to the resonance spectrum of the upside-down potential. For this reason, we expect there to be some form of monodromy in the upside-down champagne bottle potential.

# Chapter 1

# Preliminaries from Quantum Mechanics

## 1.1 Basics

Suppose there is a particle of mass $m$ moving in one dimension[1]. Given the initial position and velocity of the particle, its classical motion is completely determined by Newton's law, which reads

$$m\ddot{x} = F(x,t). \tag{1.1}$$

Here, $F(x,t)$ is the net force acting on the particle at a certain time $t$ when it is located at position $x$.

Alternatively, we can go to Hamiltonian formalism of classical mechanics. We assign to each system a Hamiltonian function $H$. This function determines how the (generalised) position and momentum of the particle change in time:

$$\begin{cases} \dot{x} = \frac{\partial H}{\partial p} \\ \dot{p} = -\frac{\partial H}{\partial x}. \end{cases} \tag{1.2}$$

We will say some more about Hamiltonian mechanics in the next chapter. Specifying the initial position and momentum completely determines the motion of the particle.

In quantum mechanics, the Hamiltonian is promoted to an operator, denoted by $\hat{H}$. A particle is described in terms of its wavefunction $\Psi(x,t)$, which is an element of a complex Hilbert space (usually $L^2$). The time evolution of the wavefunction is determined by the Schrödinger equation

$$i\hbar\frac{\partial \Psi}{\partial t} = \hat{H}\Psi. \tag{1.3}$$

When an initial wavefunction $\Psi(x,0)$ is specified, equation (1.3) determines the wavefunction of the particle for all future times.

[1]Most of the theory in this chapter is derived from [9].

The square of the wavefunction $|\Psi(x,t)|^2$ has the interpretation of a probability density function. More specifically, the probability of finding the particle between two points $a$ and $b$ when measuring at time $t$ is given by

$$\int_a^b |\Psi(x,t)|^2 \, \mathrm{d}x. \tag{1.4}$$

For this interpretation to make sense, we should require that

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, \mathrm{d}x = 1, \tag{1.5}$$

which is called normalisation of the wavefunction.

### 1.1.1 Solving the Schrödinger equation

In many cases, the Hamiltonian will be equal to the sum of the kinetic and potential energy of the particle, i.e.

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x).$$

Here, $\hat{p}$ is the momentum operator, which in quantum mechanics is defined as

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}.$$

Thus, the Schrödinger equation (1.3) reads as

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi. \tag{1.6}$$

The goal now is to determine the wavefunction of a particle moving in a specified time-independent potential $V(x)$ for all times $t > 0$. We shall look for separable solutions of the form $\Psi(x,t) = \psi(x) \cdot \phi(t)$. Substituting this into (1.6) yields:

$$i\hbar \frac{1}{\phi} \frac{\mathrm{d}\phi}{\mathrm{d}t} = -\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x).$$

The left hand side of this equation depends only on time, while the right hand side only depends on space. This implies that both expressions are constant, independent of both $x$ and $t$. The separation constant is called $E$, for reasons that will become clear later. Thus, we have separated the Schrödinger equation into two independent ordinary differential equations.

The $\phi$-equation is very simple:

$$i\hbar \frac{1}{\phi} \frac{\mathrm{d}\phi}{\mathrm{d}t} = E \implies \phi(t) = e^{-iEt/\hbar}. \tag{1.7}$$

Note that $\phi$ is independent of the potential. To solve the $\psi-$equation,

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi = E\psi, \tag{1.8}$$

a potential needs to be specified. Equation (1.8) is called the time independent Schrödinger equation. In many cases, we will refer to $\psi$ as the wavefunction, when the time dependence is clear.

Equation (1.8) may also be written in the form

$$\hat{H}\psi = E\psi, \tag{1.9}$$

so that finding the allowed energies of a system comes down to determining the spectrum of an operator. The eigenstates $\psi$ are usually called stationary states. When the particle is in such a state, the full wavefunction

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$

depends on time, but the probability density

$$|\Psi(x,t)|^2 = |\psi(x)|^2$$

does not. Moreover, the stationary states have definite energy $E$, which is also independent of time. To see this, we can compute the expected value of the Hamiltonian as

$$\begin{aligned}\langle\hat{H}\rangle &= \int_{-\infty}^{\infty} \bar{\psi}(x)\hat{H}\psi(x)\,\mathrm{d}x \\ &= \int_{-\infty}^{\infty} E\cdot|\psi(x)|^2\,\mathrm{d}x = E,\end{aligned}$$

due to normalisation. For this reason, the separation constant was called $E$.

As an example, consider the simplest possible quantum system: the particle in a box. The potential is given by

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < a \\ \infty & \text{otherwise,} \end{cases} \tag{1.10}$$

which corresponds to a particle that is free to move between $x = 0$ and $x = a$, but can not escape this region. Outside of the potential well, $\psi(x) = 0$, since the probability of finding the particle there is zero. We can find $\psi(x)$ by solving equation (1.8), which inside the well reads

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi,$$

or by substituting $k = \sqrt{2mE}/\hbar$,

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + k^2\psi = 0. \tag{1.11}$$

To make the wavefunction continuous, we impose the boundary conditions $\psi(0) = 0 = \psi(a)$. The general solution to equation (1.11) is

$$\psi(x) = A\cos(kx) + B\sin(kx).$$

Filling in the boundary conditions gives

$$\begin{aligned}\psi(0) &= A = 0\\ \psi(a) &= B\sin(ka) = 0 \implies k_n a = n\pi,\end{aligned}$$

with $n \in \mathbb{N}$. Thus, the allowed energies are

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}, \tag{1.12}$$

with corresponding stationary states

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right). \tag{1.13}$$

The pre-factor $\sqrt{2/a}$ is just a normalisation constant. To find the general solution to the time-dependent Schrödinger equation, we can simply add in the time-dependence according to equation (1.7). The general solution is then a linear combination of all stationary states:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \cdot \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\cdot e^{-\frac{iE_n t}{\hbar}} \tag{1.14}$$

Given some initial wavefunction $\Psi(x,0)$, we can find the coefficients $c_n$ by using Fourier series:

$$c_n = \sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\cdot\Psi(x,0)\,\mathrm{d}x.$$

Finally, we introduce the standard Dirac notation of quantum mechanics. A state vector in Hilbert space is often written as $|\psi\rangle$. Its dual vector is then denoted by $\langle\psi|$. We will write inner products between two states as follows:

$$\langle\phi|\psi\rangle = \int \overline{\phi(x)}\psi(x)\,\mathrm{d}x.$$

The expected value of an operator $\hat{Q}$ in a certain state $|\psi\rangle$ is then

$$\langle\hat{Q}\rangle = \langle\psi|\hat{Q}\psi\rangle.$$

## 1.2 Perturbation Theory

For a generic potential $V(x)$, equation (1.8) is difficult, or even impossible to solve. Exact values for the allowed energies can only be computed for very simple potentials, such as the infinite square well, or the harmonic oscillator.

In many practical cases, the potential $V(x)$ can be written as the sum of a simple potential $V_0(x)$, for which the exact energies are known, and a small perturbation. For example, any potential with a local minimum can be approximated by the harmonic oscillator in the neighbourhood of the minimum. Perturbation theory is a technique for dealing with small variations on known potentials.

Suppose that we have already solved the time-independent Schrödinger equation (1.8) for some potential:

$$\hat{H}^0\psi_n^0 = E_n^0\psi_n^0, \tag{1.15}$$

for some properly normalised and mutually orthogonal eigenstates $\psi_n^0$ of $\hat{H}^0$. Note that we will often omit the hat on operators when it is clear from context what is meant. We can write the perturbed Hamiltonian in the form

$$H = H^0 + \lambda H'. \tag{1.16}$$

Since the perturbation is small compared to $H^0$, we can expand the true eigenvalues and stationary states as

$$\begin{aligned}\psi_n &= \psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \mathcal{O}(\lambda^3)\\ E_n &= E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \mathcal{O}(\lambda^3).\end{aligned}$$

Substituting this into equation (1.16) and collecting orders of $\lambda$ gives, up to first order in $\lambda$,

$$H^0\psi_n^1 + H'\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0. \tag{1.17}$$

Taking inner products with $\psi_n^0$ and using the fact that $H^0$ is Hermitian[2] gives:

$$E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle. \tag{1.18}$$

This equation gives the first order correction to the energy eigenvalue of the unperturbed Hamiltonian. It has a very nice interpretation: The first order correction to the energy is the expected value of the perturbation in the unperturbed state. Moreover, the first order correction to the eigenstates can be found as:

$$\psi_n^1 = \sum_{m\neq n}\frac{\langle\psi_m^0|H'|\psi_n^0\rangle}{E_n^0 - E_m^0}\psi_m^0. \tag{1.19}$$

Note that this fraction is only defined if the system is non-degenerate, i.e. all unperturbed eigenstates have distinct energies. If there is a degeneracy in the system, we need

[2]An operator $\hat{Q}$ is Hermitian if $\langle\hat{Q}\psi|\phi\rangle = \langle\psi|\hat{Q}\phi\rangle$. Note that this justifies the notation $\langle\psi|\hat{Q}|\phi\rangle$ used below.

to resort to a different flavour of perturbation theory. As a simple example, let us consider an unperturbed Hamiltonian with a two-fold degeneracy:

$$H^0\psi_a^0 = E^0\psi_a^0, \quad H^0\psi_b^0 = E^0\psi_b^0, \tag{1.20}$$

with $\psi_a^0$ and $\psi_b^0$ normalised and orthogonal. The generalisation to an $n$-th order degeneracy will be straightforward.

Note that any linear combination of the two states

$$\psi^0 = \alpha\psi_a^0 + \beta\psi_b^0$$

is again an eigenstate of $H^0$ with the same energy. For the moment, we can keep $\alpha$ and $\beta$ variable. As before, we write $H = H^0 + \lambda H'$, and expand everything in terms of $\lambda$. To first order in $\lambda$, we get (using equation (1.17))

$$H^0\psi^1 + H'\psi^0 = E^0\psi^1 + E^1\psi^0.$$

Taking inner products with $\psi_a$ gives:

$$\alpha\langle\psi_a^0|H'|\psi_a^0\rangle = \beta\langle\psi_a^0|H'|\psi_b^0\rangle = \alpha E^1.$$

In a similar way, we can take the inner product with $\psi_b^0$ to get

$$\alpha\langle\psi_b^0|H'|\psi_a^0\rangle = \beta\langle\psi_b^0|H'|\psi_b^0\rangle = \beta E^1.$$

These two equations can be written in a compact way as a matrix-vector system:

$$\begin{pmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \tag{1.21}$$

where

$$W_{ij} = \langle\psi_i^0|H'|\psi_j^0\rangle, \quad i,j = a,b.$$

The eigenvalues of $W = (W_{ij})$ determine the first-order corrections to the energy. Notice that symmetry of the inner product implies that $W$ is a real symmetric matrix. Thus, its eigenvalues will always be real numbers.

For a general $n-$fold degeneracy, equation (1.21) will generalise in the obvious way to

$$W\vec{\alpha} = E^1\vec{\alpha}, \tag{1.22}$$

where

$$W_{ij} = \langle\psi_i^0|H'|\psi_j^0\rangle, \quad \vec{\alpha} = (\alpha_1, ..., \alpha_n).$$

## 1.3 The WKB-Method

Another technique for obtaining approximate solutions to the Schrödinger equation is the so called WKB-method, named after Wentzel, Kramer and Brillouin. This approximation scheme is based on the wavefunction of a free particle ($E > V$)

$$\psi(x) = Ae^{\pm ikx}, \quad k = \sqrt{2m(E-V)}/\hbar.$$

The sign of this equation indicates the direction in which the particle is travelling. Now, when we consider a potential that is not constant, but very close to constant, it is reasonable to assume that the wavefunction keeps this form. What changes is that $A$ and $k$ become slowly varying functions of $x$.

### 1.3.1 Deriving the Method

We can rewrite the time-independent Schrödinger equation (1.8) in the following way:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{p^2}{\hbar^2}\psi, \quad p(x) = \sqrt{2m(E-V(x))}. \tag{1.23}$$

The function $p(x)$ is the classical momentum of the particle, which is a real valued function, if we assume that $E > V$ everywhere. As described above, we try a solution of the form

$$\psi(x) = A(x)e^{i\phi(x)}.$$

Substitution gives

$$A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A.$$

Now, we can equate the real and imaginary parts, to get two equations, which are fully equivalent to the original Schrödinger equation:

$$\begin{cases} A'' = A\left((\phi')^2 - \frac{p^2}{\hbar^2}\right) \\ (A^2\phi')' = 0. \end{cases} \tag{1.24}$$

The second equation has a solution of the form

$$A = \frac{C}{\sqrt{\phi'}}. \tag{1.25}$$

For the first equation, we argue that if the potential $V(x)$ varies slowly, we can neglect the term involving $A''$. With this approximation, the first part of equation (1.24) reduces to

$$\frac{\mathrm{d}\phi}{\mathrm{d}x} = \pm\frac{p}{\hbar},$$

so that

$$\phi(x) = \frac{1}{\hbar}\int p(x)\ \mathrm{d}x$$

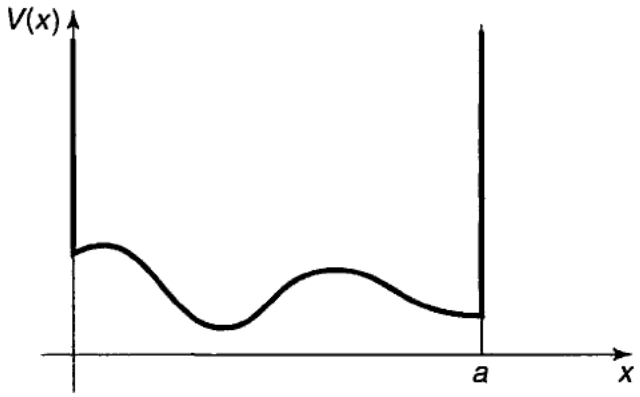



Figure 1.1: The infinite square well with a bumpy bottom. Figure from [9].

and

$$\psi(x) \approx \frac{C}{\sqrt{p(x)}} e^{\pm \frac{i}{\hbar} \int p(x)\, \mathrm{d}x}. \tag{1.26}$$

As an example, consider the infinite square well with a bumpy bottom. An example of such a potential can be seen in Figure 1.1. If $E > V(x)$ inside the well, we get from equation (1.26) that

$$\psi(x) \approx \frac{1}{\sqrt{p(x)}} \left( C_+ e^{i\phi(x)} + C_- e^{-i\phi(x)} \right) = \frac{1}{\sqrt{p(x)}} \Big( C_1 \cos(\phi(x)) + C_2 \sin(\phi(x)) \Big),$$

where

$$\phi(x) = \int_0^x p(\xi)\, \mathrm{d}\xi.$$

By continuity of the wavefunction at the barrier, we have that $\psi(0)$ must be zero. Using that $\phi(0) = 0$ gives $C_2 = 0$. At the other end of the well, we must also have $\psi(a) = 0$. Thus,

$$\phi(a) = \frac{1}{\hbar} \int_0^a p(x)\, \mathrm{d}x = n\pi. \tag{1.27}$$

An equation like this is called a quantisation condition. The term $\int p\ \mathrm{d}x$ is known in classical mechanics as an action variable. We shall encounter these later when we study the champagne bottle potential.

When $E < V(x)$, tunnelling becomes possible. In this regime, the wavefunction of the free particle is of the form

$$\psi(x) = A e^{\pm \kappa x}.$$

When $V(x)$ varies slowly, we can use the same argument as before to show that

$$\psi(x) \approx \frac{C}{\sqrt{|p(x)|}} e^{\pm \frac{1}{\hbar} \int |p(x)|\, \mathrm{d}x}. \tag{1.28}$$

### 1.3.2 The Connection Formulae

If the walls of the potential well are vertical, the boundary conditions are quite trivial, and it is easy to write down the quantisation condition. In this section, we want to study what happens near a classical turning point ($E = V(x)$), where the WKB-approximation breaks down. The goal is to derive a quantisation condition similar to equation (1.27) using so-called connection formulae.

For simplicity, consider a potential that has a turning point at $x = 0$. Suppose that the slope of the potential is positive at the turning point. Then, by the WKB method, we have that

$$\psi(x) \approx \begin{cases} \frac{1}{\sqrt{p(x)}} \left[ B e^{\frac{i}{\hbar}\int_x^0 p(\xi)\mathrm{d}\xi} + C e^{-\frac{i}{\hbar}\int_x^0 p(\xi)\mathrm{d}\xi} \right] & (x < 0) \\ \frac{1}{\sqrt{|p(x)|}} D e^{-\frac{1}{\hbar}\int_0^x |p(\xi)|\mathrm{d}\xi} & (x > 0). \end{cases} \tag{1.29}$$

Here, we can set $B = 0$, since this term blows up for large $x$. These two solutions need to be joined up at $x = 0$. The problem is that when $x \to 0$, also $p(x) \to 0$. Hence, near the turning point $\psi(x) \to \infty$. We will need to find a patching wavefunction $\psi_p$ near the turning point to glue the different parts together.

Since we only need the patching wavefunction in a small neighbourhood of the turning point, we can obtain an approximation by linearising the potential about $x = 0$, and solving the Schrödinger equation:

$$V(x) \approx E + V'(0)x.$$

Substituting

$$\alpha = \sqrt[3]{\frac{2m}{\hbar^2} V'(0)}$$

leads to

$$\frac{\mathrm{d}^2\psi_p}{\mathrm{d}x^2} = \alpha^3 x \psi_p.$$

Moreover, we can set $z = \alpha x$. This yields

$$\frac{\mathrm{d}^2\psi_p}{\mathrm{d}z^2} = z\psi_p, \tag{1.30}$$

which is known in the literature as Airy's equation. The solutions can be represented as a linear combination of the Airy functions

$$\psi_p(z) = a\,\mathrm{Ai}(z) + b\,\mathrm{Bi}(z).$$

Some properties of these special function, and their asymptotic forms can be found in [1].

The wavefunction $\psi_p$ is a good approximation of the true wavefunction close to the classical turning point, while the WKB-method works well far away from the turning point. To glue the two approximations together, we need to consider what happens in the overlap region, where both approximations reflect the true wavefunction reasonably well. Substituting the linearisation into the definition of $p(x)$ yields:

$$p(x) \approx \sqrt{2m(E - E - V'(0)x)} = \hbar\alpha^{3/2}\sqrt{-x}.$$

Hence, in overlap region 2, we can write

$$\int_0^x |p(\xi)| \, \mathrm{d}\xi \approx \hbar\alpha^{3/2} \int_0^x \sqrt{\xi} \, \mathrm{d}\xi = \frac{2}{3}\hbar(\alpha x)^{3/2}.$$

Plugging this expression into the WKB-wavefunction from equation (1.29) gives

$$\psi(x) \approx \frac{D}{\sqrt{\hbar}\alpha^{3/4}x^{1/4}} e^{-\frac{2}{3}(\alpha x)^{3/2}}. \tag{1.31}$$

Near the turning point, we can use the large$-z$ asymptotic form of the Airy functions to get

$$\psi_p(x) \approx \frac{a}{2\sqrt{\pi}(\alpha x)^{1/4}} e^{-\frac{2}{3}(\alpha x)^{3/2}} + \frac{b}{\sqrt{\pi}(\alpha x)^{1/4}} e^{\frac{2}{3}(\alpha x)^{3/2}} \tag{1.32}$$

Comparing coefficients in equations (1.31) and (1.32) yields

$$a = \sqrt{\frac{4\pi}{\alpha\hbar}} D, \quad b = 0.$$

A similar derivation can be done in the other overlap region. For the full details, see [9]. We can now write down the connection formulae, which join together the WKB-wavefunctions at both sides of the turning point. If we shift this point back to an arbitrary point $x_2$, we get

$$\psi(x) \approx \begin{cases} \frac{2D}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_x^{x_2} p(\xi) \, \mathrm{d}\xi + \frac{\pi}{4}\right) & x < x_2 \\ \frac{D}{\sqrt{|p(x)|}} \exp\left(-\frac{1}{\hbar}\int_{x_2}^x |p(\xi)| \, \mathrm{d}\xi\right) & x > x_2. \end{cases} \tag{1.33}$$

We are now in a position to write down a quantisation condition like equation (1.27) for a potential well with 1 vertical wall, say at $x = 0$. An example of a potential like this can be seen in Figure 1.2. From continuity of the wavefunction at $x = 0$, we get that $\psi(0) = 0$. Hence, equation (1.33) reads

$$\frac{1}{\hbar}\int_0^{x_2} p(x) \, \mathrm{d}x + \frac{\pi}{4} = n\pi, \quad n = 1, 2, ...$$

The proper quantisation condition is thus

$$\int_0^{x_2} p(x) \, \mathrm{d}x = \left(n - \frac{1}{4}\right)\pi\hbar. \tag{1.34}$$

However, in most practical cases, the potential will have no vertical walls. This case needs to be handled with special care. Consider a single potential well. We already know what happens near the right turning point, since the potential has a positive slope here. At the left turning point, the connection formulae are given by

$$\psi(x) \approx \begin{cases} \frac{D'}{\sqrt{|p(x)|}} \exp\left(-\frac{1}{\hbar}\int_x^{x_1} |p(\xi)| \, \mathrm{d}\xi\right), & x < x_1, \\ \frac{2D'}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_{x_1}^x p(\xi) \, \mathrm{d}\xi + \frac{\pi}{4}\right), & x > x_1 \end{cases} \tag{1.35}$$

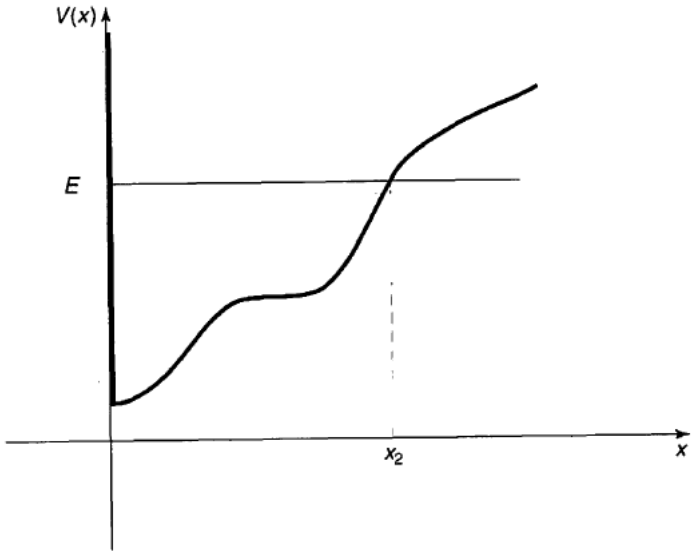



Figure 1.2: A potential well with one vertical wall. Figure from [9].

Inside the potential well, equations (1.33) and (1.35) describe the same wavefunction. Hence, they must be equal inside the well. We get that

$$\frac{2D'}{\sqrt{p(x)}} \sin\theta_1(x) = \frac{2D}{\sqrt{p(x)}} \sin\theta_2(x)$$

with

$$\theta_1(x) = \frac{1}{\hbar}\int_{x_1}^{x} p(\xi)\,\mathrm{d}\xi + \frac{\pi}{4}, \quad \theta_2(x) = \frac{1}{\hbar}\int_{x}^{x_2} p(\xi)\,\mathrm{d}\xi + \frac{\pi}{4}.$$

If the sine functions must agree for all values of $x$, then clearly their argument must differ by an integer multiple of $\pi$. Hence, the quantisation condition is

$$\int_{x_1}^{x_2} p(x)\,\mathrm{d}x = \left(n - \frac{1}{2}\right)\pi\hbar, \quad n = 1, 2, ... \tag{1.36}$$

This condition determines all allowed energies of the particle, without the need to solve the Schrödinger equation.

# Chapter 2

# The Champagne Bottle Potential

In this chapter, we will look at both the classical and quantum monodromy in the champagne bottle potential. A plot of this potential can be seen in Figure 2.1. We will first develop part of the mathematical framework of classical mechanics, including the theory of action-angle variables. We will then apply this framework to the champagne bottle potential. Doing so will show that there is both classical and quantum monodromy in this system.

## 2.1 Theoretical Framework

Mathematically speaking, a Hamiltonian system consists of three parts: The phase space $X$, a $2n$-dimensional manifold; a symplectic structure[1] $\omega$ on $X$; and a real-valued function $H$ defined on $X$, which is called the Hamiltonian of the system.

Time evolution of the system is determined by Poisson brackets. For any function $f$

[1] A symplectic form is an abstract object that allows you to measure two-dimensional objects in the space $X$.

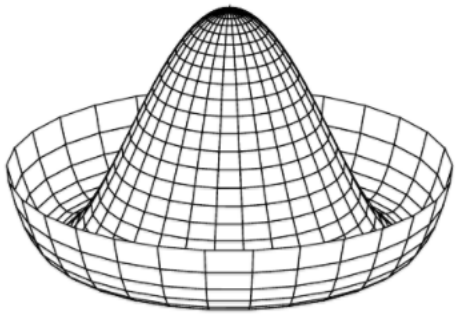


Figure 2.1: Visual representation of the champagne bottle potential, which we will study in this chapter.

dependent on time and space, we have that

$$\frac{\mathrm{d}f(x,t)}{\mathrm{d}t} = \{f, H\} + \frac{\partial f}{\partial t}.$$

We call a system completely integrable if there exist functions $f_1, ..., f_n$ whose Poisson brackets vanish, and which are independent in the sense that $\mathrm{d}f_i$ are linearly independent almost everywhere. Physically, this means that there are as many conserved quantities as there are degrees of freedom. Usually, one of the $f_i$ can be taken as the Hamiltonian function itself.

For any completely integrable system, we can define the map

$$F : X \to \mathbb{R}^n, \quad F(x) = (f_1(x), ..., f_n(x)). \tag{2.1}$$

Define $B = F(X)$, and for $c \in B$, let $F_c$ be the level set of $F$ corresponding to the value $c$. Since the values of all $f_i$ are conserved quantities, trajectories will live on these level sets. Generally, we will assume that each $F_c$ is compact and connected.

Locally, the structure of completely integrable systems is described by the Arnold-Liouville theorem. A proof of this theorem can be found in [2].

**Theorem** (Arnold-Liouville)**.** *Let $c \in B$ be a regular value of a completely integrable system $F = (f_1, ..., f_n) : X \to B$, and let $F_c = F^{-1}(\{c\})$. Then, $F_c$ is a Lagrangian submanifold of $X$*[2]*. Furthermore, suppose that $F_c$ is compact and connected. Then, there is a neighbourhood $U$ of $F_c$ in $X$ and a diffeomorphism $(I, \alpha) : U \to V \times \mathbb{T}^n$, where $V$ is an open subset of $\mathbb{R}^n$ and $\mathbb{T}^n$ is a torus $\mathbb{S}^1 \times ... \times \mathbb{S}^1$, such that $(I, \alpha)$ are symplectic coordinates, and $F$ is a function of $I$ only.*

The coordinates $(I, \alpha)$ are called action-angle variables of the system. As described in [11], the actions are given by

$$I = \frac{1}{2\pi} \oint p \, \mathrm{d}q, \tag{2.2}$$

where the integration path is a closed trajectory. It follows from canonical transformation theory that the angle variable $\alpha$ can now be computed as

$$\alpha(q, I) = \sqrt{\frac{m}{2}} \left( \frac{\partial \tilde{H}}{\partial I} \right) \int^q \sqrt{2m(\tilde{H}(I) - V(q))} \, \mathrm{d}q^3. \tag{2.3}$$

The lower limit of the integral is a free parameter. All it does is induce a phase convention in the system. Often, a smart choice of this limit can simplify the problem.

As an example, consider the simple harmonic oscillator. The Hamiltonian of this system is given by

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2. \tag{2.4}$$

[2] A Lagrangian submanifold $L \subset X$ is an $n$-dimensional submanifold of $X$ satisfying $\omega|_L = 0$.

[3] For an overview of this theory, see for example [5].

The value of this Hamiltonian on a trajectory is denoted by $E$. To compute the action, we have to evaluate equation (2.2). The momentum $p$ can be solved from equation (2.4):

$$\begin{aligned} p &= \sqrt{2mE - m^2\omega^2 q^2} \\ &= \sqrt{m^2\omega^2 \left(\frac{2E}{m\omega^2} - q^2\right)} \\ &= m\omega\sqrt{q_0^2 - q^2}, \quad \text{where} \quad q_0 := \frac{1}{\omega}\sqrt{\frac{2E}{m}}. \end{aligned}$$

Now, the turning points are located at $\pm q_0$ so that the action is given by

$$\begin{aligned} I &= \frac{m\omega}{2\pi} \oint \sqrt{q_0^2 - q^2}\, \mathrm{d}q \\ &= \frac{m\omega}{\pi} \int_{-q_0}^{q_0} \sqrt{q_0^2 - q^2}\, \mathrm{d}q \\ &= \frac{1}{2} m\omega q_0^2 \\ &= \frac{E}{\omega}. \end{aligned}$$

Notice that the transformed Hamiltonian $\tilde{H}(I) = I\omega$ is indeed a function of the action only. Next, we must relate the angle coordinate $\alpha$ to the original coordinates $(p, q)$. Choosing $q_0$ as the limit in equation (2.3) gives

$$\begin{aligned} \alpha &= \sqrt{\frac{m\omega^2}{2}} \int_q^{q_0} \sqrt{I\omega - \frac{1}{2}m\omega^2 q^2}\, \mathrm{d}q \\ &= \int_q^{q_0} \frac{\mathrm{d}q}{\sqrt{q_0^2 - q^2}} \\ &= \arccos(q/q_0). \end{aligned}$$

Thus, the transformation is given by

$$\begin{cases} q = \sqrt{2I/m\omega}\cos\alpha, \\ p = -\sqrt{2Im\omega}\sin\alpha. \end{cases}$$

For a quantum-mechanical system, the action-angle variables are used in semi-classical quantisation. In general, the Bohr-Sommerfeld rule says that

$$\frac{1}{2\pi} \oint p\, \mathrm{d}q = (n - \delta)\hbar, \tag{2.5}$$

for an appropriate phase angle $\delta$[5]. As seen in the previous chapter, a potential well with no vertical walls has a phase angle $\delta = 1/2$. Alternatively, this can be seen as a quantisation condition for the action $I$. This relation gives the correct energy eigenvalues in the limit $\hbar \to 0$, hence the name semi-classical quantisation.

## 2.2 Classical Monodromy in the Champagne Bottle

We will now look at classical monodromy in the champagne bottle potential. In general, the word monodromy is used to describe what happens to objects as they run around a singularity. An example of this could be the complex logarithm, which changes by $2\pi i$ each time we traverse the unit circle. We will see what monodromy means in the context of classical and quantum mechanical systems.

Consider a point particle of mass $m = 1$ moving through a potential in the plane defined by

$$V(r) = r^4 - r^2, \tag{2.6}$$

with $r^2 = x^2 + y^2$. We write the Hamiltonian of this system in polar coordinates as

$$H = \frac{1}{2}(p_r^2 + \frac{p_\theta^2}{r^2}) + r^4 - r^2. \tag{2.7}$$

Since the Hamiltonian is independent of the coordinate $\theta$, we have that its conjugate momentum $p_\theta = L$ is conserved throughout the motion of the particle. Also, the total energy $H = E$ is a conserved quantity. We thus have as many conserved quantities as there are degrees of freedom, meaning that this system is completely integrable.

Next, consider a mapping $F : \mathbb{R}^4 \to \mathbb{R}^2$, which maps a point in phase space $(x, y, p_x, p_y)$ to the values of $E$ and $L$ at that point. To apply the Arnold-Liouville theorem, we will first need to compute the critical values, and thus the regular values of $F$.

Since we are using polar coordinates, we will treat the case $x = y = 0$ separately. Note that in this case, we have that

$$\begin{aligned} \mathrm{d}E &= p_x \mathrm{d}p_x + p_y \mathrm{d}p_y, \\ \mathrm{d}L &= p_x \mathrm{d}y - p_y \mathrm{d}x, \end{aligned}$$

so that

$$\mathrm{d}E \wedge \mathrm{d}L = 0 \quad \iff p_x = p_y = 0.$$

Therefore, $(E, L) = (0, 0)$ is a critical value of $F$. If either $x$ or $y$ is non-zero, $r \neq 0$. In this case,

$$\begin{aligned} \mathrm{d}E &= p_r \mathrm{d}p_r + \frac{1}{r^2} p_\theta \mathrm{d}p_\theta + \left(4r^3 - 2r - \frac{p_\theta^2}{r^3}\right) \mathrm{d}r, \\ \mathrm{d}L &= \mathrm{d}p_\theta. \end{aligned}$$

We can see from these expressions that the rank of $\mathrm{d}E \wedge \mathrm{d}L$ is less than 2 if $p_r = 0$ and

$$p_\theta^2 = 4r^6 - 2r^4. \tag{2.8}$$

This type of critical value can only occur if the right-hand-side of this equation is positive, which is when $r > 1/\sqrt{2}$. Substitution into equation (2.7) yields that the critical values of the map $F$ are given by (0,0), and the curve parametrised by

$$(E, L) = (3r^4 - 2r^2, \pm\sqrt{4r^6 - 2r^4}), \quad r > \frac{1}{\sqrt{2}}.$$

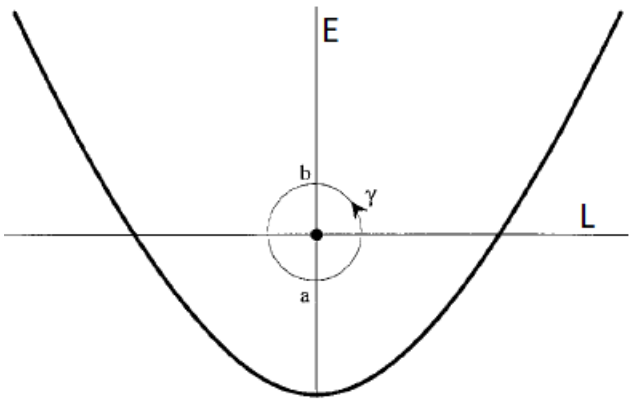



Figure 2.2: Thick black lines represent the critical values of $F$. Horizontal $L$, vertical $E$. The image of $X$ under $F$ is the region above the black curve. Everything below it is forbidden. To show that there is monodromy in the system, we will parallel transport the actions around the integration path $\gamma$.

A plot of the critical values is given in Figure 2.2. The point (0,0) corresponds physically to the particle laying still at the unstable equilibrium, or asymptotically moving towards it. The regular values of $F$ are hence all points above the black curve, excluding the origin.

Let $R$ denote the set of all regular values of $F$. It is possible to show that $F^{-1}(c)$ is connected and compact for any regular value $c \in R$. Hence, by the Arnold-Liouville theorem, $F^{-1}(c)$ is diffeomorphic to a torus for any $c \in R$. To understand the classical monodromy in the system, we need to understand the global structure of this torus bundle.

As a first step, we will investigate the energy surfaces of the system. We will distinguish the cases $E > 0$ and $E < 0$. Consider a particle moving in the champagne bottle potential with small angular momentum $L$. Fixing an energy below zero implies that the particle cannot cross the potential barrier. When the $E$ is above zero, the particle has enough energy to go over the barrier. This behaviour can be seen in Figure 2.3. When the sign of $E$ changes from negative to positive, the topology of the energy surface changes from $\mathbb{S}^2 \times \mathbb{S}^1$ to $\mathbb{S}^3$. This change in topology as we pass through a critical value hints at the fact that there is monodromy in the system. We call this rule of thumb Cushman's principle. [8].

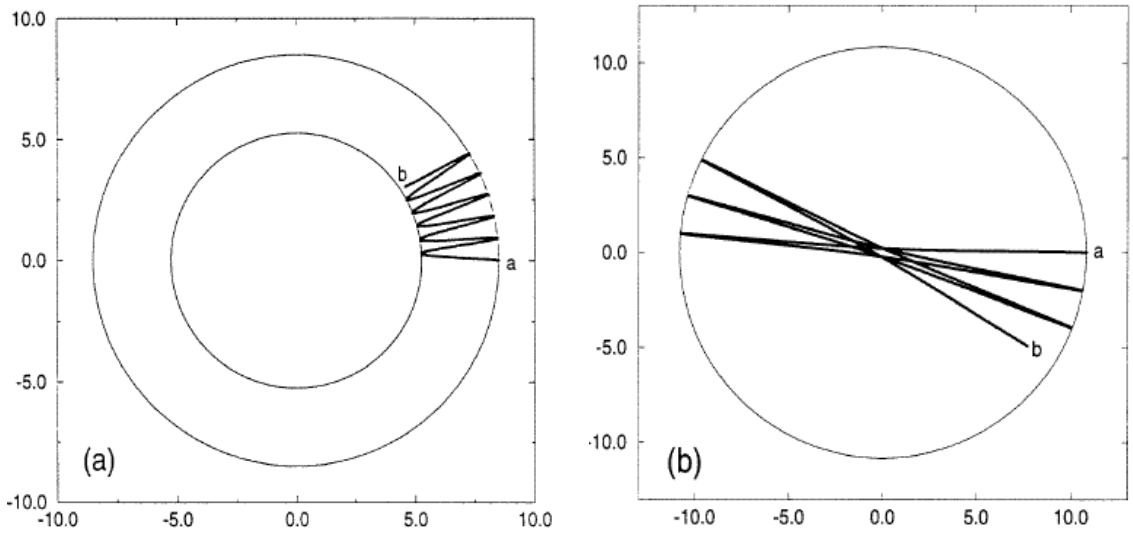
A formal proof of the monodromy requires investigating the action-angle variables of the system. These are given by

$$\begin{cases} I_\theta^\pm = \frac{1}{2\pi} \oint p_\theta \, \mathrm{d}\theta = L, \\ I_r^\pm = \frac{1}{2\pi} \oint p_r \, \mathrm{d}r = \frac{1}{\pi} \int_{r_{min}}^{r_{max}} p_r \, \mathrm{d}r, \end{cases} \tag{2.9}$$

where

$$p_r = \sqrt{2m\left(E + r^2 - r^4 - \frac{L^2}{2mr^2}\right)},$$

and $r_{min}, r_{max}$ are the classical turning points. Moreover, the $+$ and $-$ refer to division of the set of regular values $R$ into subsets where $L$ is positive, respectively negative. The




(a) Motion when $E < 0$.

(b) Motion when $E > 0$.

Figure 2.3: The topology of the energy surface changes from $\mathbb{S}^2 \times \mathbb{S}^1$ to $\mathbb{S}^3$ as the sign of the energy changes.

monodromy is computed by parallel transporting a tangent vector $\delta I = (\delta I_\theta, \delta I_r)$ around the critical value at the origin. As shown in Bates [4], the monodromy matrix is

$$M = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}.$$

Since this matrix has a non-zero off diagonal entry, there is monodromy in the system. A consequence of this is that there is no way to globally define action-angle variables.

## 2.3 The Quantum Mechanical Spectrum

As discussed in section 1.3, we can obtain the semi-classical limit of the spectrum by quantising the actions:

$$I_\theta = \frac{1}{2\pi} \oint p_\theta \, \mathrm{d}\theta = \ell\hbar, \tag{2.10}$$

$$I_r = \frac{1}{2\pi} \oint p_r \, \mathrm{d}r = \left(v - \frac{1}{2}\right)\hbar, \tag{2.11}$$

where $\ell$ and $v$ are the quantum numbers of the system. Alternatively, we could introduce the label

$$I_n = 2I_r + |I_\theta| = (2v + |\ell| + 1)\hbar = (n+1)\hbar.$$

Both labels $|v, \ell\rangle$ and $|n, \ell\rangle$ give the same description of the system.

To obtain qualitative results, we first introduce the parameters $a$ and $b$ in the Hamiltonian:

$$H = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2}\right) - ar^2 + br^4.$$

Moreover, we will adopt the following scaling:

$$\rho = \sqrt[4]{\frac{\hbar^2}{2ma}}r, \quad E = \frac{2a\hbar^2}{m}\epsilon, \quad b = \sqrt[4]{\frac{8ma^3}{\hbar^2}}\beta, \tag{2.12}$$

so that the scaled Hamiltonian becomes

$$\hat{h} = -\frac{1}{2}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) - \frac{\ell^2}{\rho^2}\right) - \frac{1}{2}\rho^2 + \beta\rho^4. \tag{2.13}$$

The new variables $\rho, \epsilon$ and $\beta$ are all dimensionless. We will numerically determine the joint spectrum of this Hamiltonian in two different ways.

First of all, we can use the quantisation condition. With the new scaling, this can be rewritten as

$$\begin{aligned}\frac{I_r}{2\hbar} &= \int_{\rho_{min}}^{\rho_{max}} \sqrt{2\epsilon + \rho^2 - 2\beta\rho^2 - \frac{\ell^2}{\rho^2}}\,\mathrm{d}\rho \\ &= \frac{1}{2}\int_{z_{min}}^{z_{max}} \frac{\sqrt{2\epsilon z + z^2 - 2\beta z^3 - \ell^2}}{z}\,\mathrm{d}z = \left(v - \frac{1}{2}\right)\pi,\end{aligned}$$

where we have substituted $z = \rho^2$. After fixing $v$ and $\ell$, this is essentially a root-finding problem. The value of $\epsilon$ can be found by numerically computing the integral, and adjusting $\epsilon$ until the quantisation condition is met.

Another way to determine the spectrum of $\hat{h}$ is by using perturbation theory (see section 1.2). We will expand the eigenstates into a two-dimensional harmonic oscillator basis. This problem can be solved analytically, which is done in [13]. Sandev and Petreska obtain the following wavefunctions for the two-dimensional harmonic oscillator:

$$\psi_{v,\ell}(R,\phi) = \sqrt{\frac{v!}{\pi\Gamma(v+|\ell|+1)}}\frac{1}{R_0^{|\ell|+1}}e^{i\ell\phi}R^{|\ell|}e^{-\frac{1}{2}\frac{R^2}{R_0^2}}L_v^{|\ell|}\left(\frac{R^2}{R_0^2}\right), \tag{2.14}$$

where, in our conventions, $R/R_0 = \rho$. Moreover, $L_k^\alpha(z)$ are the generalised Laguerre polynomials. Some properties of these functions are given in [1].

For fixed $\ell$, the energy levels after first order correction are given by the eigenvalues of $W$, where

$$W_{mn} = \langle\psi_{m,\ell}|\hat{h}|\psi_{n,\ell}\rangle.$$

Note that when $\ell$ is fixed, $n$ and $m$ increase in steps of 2, since $v$ increases in steps of 1. This follows from the relation

$$n = 2v + |\ell|.$$

To compute the matrix elements, we have to use the recursion relations of the Laguerre polynomials.

We will split up the Hamiltonian as

$$\hat{h}\psi = \hat{t}\psi - \frac{1}{2}\rho^2\psi + \beta\rho^4\psi, \quad \hat{t} := -\frac{1}{2}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) - \frac{\ell^2}{\rho^2}\right)$$

and consider each term separately. Using the recursion relations, we can find that

$$2\hat{t}\psi_{n,\ell} = \frac{1}{2}\sqrt{(n+2)^2-\ell^2}\psi_{n+2,\ell} + (n+1)\psi_{n,\ell} + \frac{1}{2}\sqrt{n^2-\ell^2}\psi_{n-2,\ell}, \tag{2.15}$$

$$\rho^2\psi_{n,\ell} = -\frac{1}{2}\sqrt{(n+2)^2-\ell^2}\psi_{n+2,\ell} + (n+1)\psi_{n,\ell} - \frac{1}{2}\sqrt{n^2-\ell^2}\psi_{n-2,\ell}. \tag{2.16}$$

We will show how to derive the second of these relations, so that the first may be checked by the reader. Without loss of generality, we can take $\ell \geq 0$. The negative part of the spectrum can then be determined by reflecting the positive part in the vertical axis. Rewriting equation (2.14) in terms of $n$ and ignoring some constants that only depend on $\ell$ gives

$$\psi_{n,\ell} = \sqrt{\frac{2\left(\frac{n-\ell}{2}\right)!}{\pi\left(\frac{n+\ell}{2}\right)!}}\rho^\ell e^{-\frac{1}{2}\rho^2} L^\ell_{(n-\ell)/2}(\rho^2) =: N(n,\ell)\rho^\ell e^{-\frac{1}{2}\rho^2} L^\ell_{(n-\ell)/2}(\rho^2).$$

After multiplication by $\rho^2$, we will have a term of the form $zL^\alpha_k(z)$, which can be rewritten as follows:

$$zL^\alpha_k(z) = -(k+\alpha)L^\alpha_{k-1}(z) + (2k+1+\alpha)L^\alpha_k(z) - (k+1)L^\alpha_{k+1}(z).$$

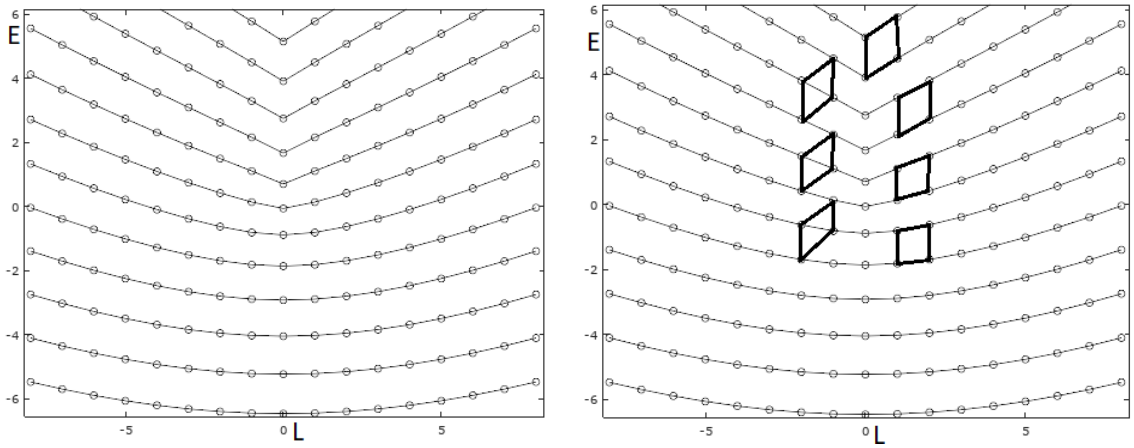
Then, we obtain

$$\begin{aligned} z\psi_{n,\ell} &= N(n,\ell)\rho^\ell e^{-\frac{1}{2}z}\left(zL^\ell_{(n-\ell)/2}(z)\right) \\ &= N(n,\ell)\rho^\ell e^{-\frac{1}{2}z}\left(\frac{n+\ell}{2}L^\ell_{(n-\ell-2)/2}(z) + (n+1)L^\ell_{(n-\ell)/2}(z) - \frac{n-\ell+2}{2}L^\ell_{(n-\ell+2)/2}(z)\right) \\ &= (n+1)\psi_{n,\ell} + \frac{n+\ell}{2}\frac{N(n,\ell)}{N(n-2,\ell)}\psi_{n-2,\ell} - \frac{n-\ell+2}{2}\frac{N(n,\ell)}{N(n+2,\ell)}\psi_{n+2,\ell}. \end{aligned}$$

Carrying out the necessary algebra will then yield the desired result. To compute a similar relation for $\rho^4$, we can simply apply this equation to itself. Note that this process introduces terms proportional to $\psi_{n+4,\ell}$ and $\psi_{n-4,\ell}$.

Now, we can compute the matrix elements by exploiting the fact that all $\psi_{n,\ell}$ are mutually orthogonal. The resulting matrix $W$ will be symmetric, and it will have 5 diagonals with non-zero elements. Its eigenvalues can be determined numerically by using MATLAB.

In the spectrum, lines have been drawn to connect eigenvalues of common quantum number $v$. As we go through the origin, the nature of these lines changes. This result is analogous to the change in topology of the energy surfaces when we considered the classical




(a) The quantum mechanical spectrum. (b) Quantum Monodromy.

Figure 2.4: The numerically determined quantum spectrum of $\hat{h}$. Horizontal $\ell$, vertical $\epsilon$. Lines connect common quantum number $v$.

case. To prove that there is actually quantum monodromy in the system, we can transport a unit grid cell around the singularity. After a full rotation, the cell is transformed in a non-trivial way. This implies that there is quantum monodromy in the champagne bottle potential. We can now conclude that there is no way to define a global grid structure on the spectrum. This result resembles the fact that there were no global action-angle variables in the classical system.

# Chapter 3

# Resonances and Complex Scaling

## 3.1 Theory

As we saw in the first chapter, a free quantum particle can be described by a plane wave. Imagine that the particle comes in on a potential barrier with two turning points. As the particle hits the first of these turning points, part of the wave is transmitted, and part is reflected. The same thing will happen at the second turning point. Hence, we see that the wave will interfere with itself in between the turning points. This will create a standing wave of a certain energy.

In some cases, the energy of this wave will correspond to one of the allowed energies of the upside-down potential. When this happens, the particle will spend a long time moving in the classically forbidden region. This is a type of resonance state.

In more generality, we can consider a scattering experiment, in which a 'particle' is scattered off a 'target'. In this context, a resonance state is defined as a long lived state of a system which has sufficient energy to break up into two or more subsystems[12].

Resonance phenomena are mainly controlled by poles of the scattering matrix. It can be

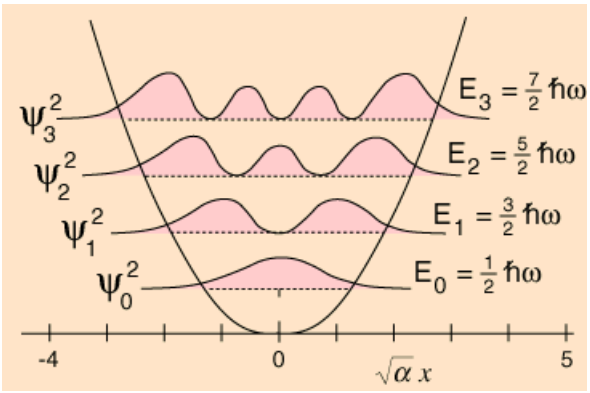



Figure 3.1: Discrete energy levels corresponding to bound states in the harmonic oscillator potential.

shown that resonance poles correspond to complex eigenvalues of the Hamiltonian operator

$$\hat{H}\phi_n^{res} = E_n\phi_n^{res}, \quad E_n = \epsilon_n - \frac{i}{2}\Gamma_n, \tag{3.1}$$

where $\epsilon_n$ is the resonance position, and $\Gamma_n$ is the inverse lifetime of the resonance, according to $\tau_n = \hbar/\Gamma_n$. Usually, we impose that $\hat{H}$ is a Hermitian operator, meaning that all of its eigenvalues are real. In this case, it is thus clear that the resonance states $\phi_n^{res}$ are not square integrable. When we add in the standard time dependence, we obtain

$$\psi_n^{res}(r,t) = \phi_n^{res}(r)e^{-iE_nt/\hbar},$$

from which it follows that the probability density

$$|\psi_n^{res}(r,t)|^2 = |\phi_n^{res}(r)|^2 e^{-\Gamma_n t/\hbar}.$$

Thus, the probability density decays exponentially to zero as time goes to infinity. Physically, this means that all incoming particles eventually disappear from any point in the coordinate space.

In order to compute the resonance spectrum of a given potential, we will introduce complex scaling. We want to make the resonance states $\phi_n^{res}$ into square integrable functions. For this, we will do a similarity transformation on the Hamiltonian. Multiplying equation (3.1) from the left by an operator $\hat{S}$ gives

$$(\hat{S}\hat{H}\hat{S}^{-1})(\hat{S}\phi_n^{res}) = \left(\epsilon_n - \frac{i}{2}\Gamma_n\right)(\hat{S}\phi_n^{res}).$$

We would thus like to impose that $\hat{S}\phi_n^{res}$ is square integrable, so that we can apply standard methods to determine the spectrum.

One way to do this, is to select

$$\hat{S}_\theta = e^{i\theta r\frac{\partial}{\partial r}},$$

such that

$$\hat{S}_\theta f(r) = f(re^{i\theta})$$

for any analytic function $f(r)$. We will call $\hat{S}$ the complex scaling operator. It is possible to show that a resonance function $\phi_n^{res}$ will become square integrable for sufficiently large values of the rotational angle $\theta$. The advantage of complex scaling is thus that it associates a resonance phenomenon to the discrete part of the spectrum of the complex scaled Hamiltonian. Moreover, the resonance state is associated to a single square integrable function. The complex scaling procedure can be viewed as compressing information about the evolution of a resonance state into a small part of space.

In some cases, it is possible to determine the resonance spectrum of a potential by studying the upside-down variant. More specifically, assume that we have an analytical expression $E(n,\lambda)$ for the discrete energy levels of a potential $V(r) = \lambda v(r)$. Assume that for $\lambda > 0$, we have a potential well that supports bound states. When we do the

transformation $\lambda \mapsto -\lambda$ to the upside-down potential, we get a barrier. If this new potential supports resonance states, then $E(n, -\lambda)$ is a complex-valued function of the quantum number $n$. The real and imaginary parts of this function are the resonance position and line width respectively.

The simplest case where this happens is the parabolic barrier potential

$$V(x) = \frac{1}{2}kx^2.$$

This problem is studied in [3] in much more detail. The eigenvalues of this potential are products of Kummer functions with decaying exponentials. Now, it can be shown that the eigenvalues of the complex-scaled Hamiltonian are given by [12]

$$E_n = -i\hbar\omega\left(n - \frac{1}{2}\right).$$

Hence, we see that the resonance positions are all zero, while the lifetime of the resonance states is given by

$$\frac{1}{\tau_n} = 2\hbar\omega\left(n - \frac{1}{2}\right).$$

This type of potential is very useful in chemistry, where the barrier between products and reactants is often modelled by a parabolic barrier potential.

## 3.2 Application to the Inverted Champagne Bottle

We would now like to apply the complex scaling method to the inverted champagne bottle potential. From the discussion in the previous section, we have seen that the resonance spectrum of a barrier is related to the spectrum of the upside-down potential. It is thus natural to expect that there is some form of monodromy in the inverted champagne bottle potential.

Similar to the normal champagne bottle, we will use a scaled model with a parameter $\beta$ to control the density of states. The scaled Hamiltonian is given by

$$\hat{h} = \hat{t} + \frac{1}{2}\rho^2 - \beta\rho^4, \tag{3.2}$$

where we recall that

$$\hat{t} = -\frac{1}{2}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) - \frac{\ell^2}{\rho^2}\right).$$

Upon complex scaling, we have that $\rho$ is mapped to $\rho e^{i\theta}$. This implies that the terms proportional to $\rho^2$ and $\rho^4$ pick up a factor $e^{2i\theta}$ and $e^{4i\theta}$ respectively. Meanwhile, the kinetic term is scaled by a factor $e^{-2i\theta}$. Hence, the complex scaled Hamiltonian is given by

$$\hat{h}_\theta = e^{-2i\theta}\hat{t} + \frac{1}{2}e^{+2i\theta}\rho^2 - \beta e^{+4i\theta}\rho^4. \tag{3.3}$$

Notice that the terms in this Hamiltonian are identical to the one of the regular champagne bottle, except for different constants. Hence, when we again expand the eigenstates into harmonic oscillator basis, we will be able to use the same inner products that were derived in the previous chapter. What changes is that the entries of $W$ will no longer be real, because of the complex exponentials in $\hat{h}_\theta$. This implies that the eigenvalues of $W$ will in general be complex numbers, with non-zero real and imaginary parts.

Using a script that is almost identical to the one used in the previous chapter, the resonance spectrum of $\hat{h}_\theta$ can be determined. First, we checked that our method reproduces the resonance spectrum of a two dimensional parabolic barrier potential. As expected, the real part of the spectrum is numerically zero, while the imaginary part has perfect grid structure. In all of these spectra, note that we have only considered eigenvalues with negative real part, since they correspond to resonance states with positive lifetime. Moreover, an eigenvalue is only included in the plot if its real part is below 20. This is to ensure that we can actually 'trust' all the determined eigenvalues.

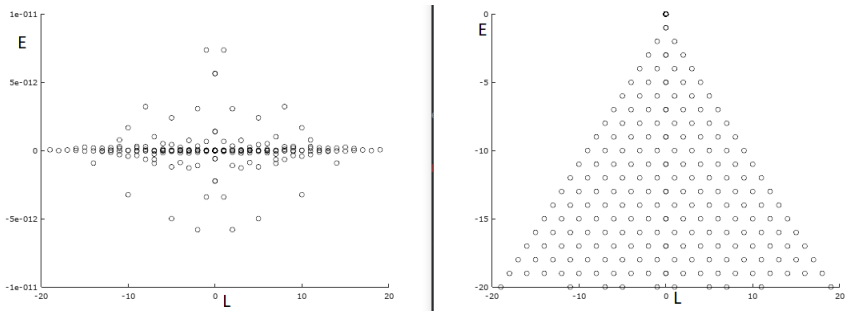



Figure 3.2: Numerical result for the two dimensional parabolic barrier, complex scaling angle $\theta = 1$. Left: real part, Right: imaginary part.

We now show some results for various values of the complex scaling angle $\theta$. When $\theta = 0.1$, the diagonal lines seem to indicate that we have not scaled down the Hamiltonian enough. For $\theta = 0.5$, these lines have vanished. However, when we increase $\theta$ further to 1, the real part of the spectrum flips through the origin. This is not a good sign, since we are looking for features of the spectrum that are independent of both the complex scaling angle and the matrix size. We were thus unable to confirm if there is monodromy in the system using this method.

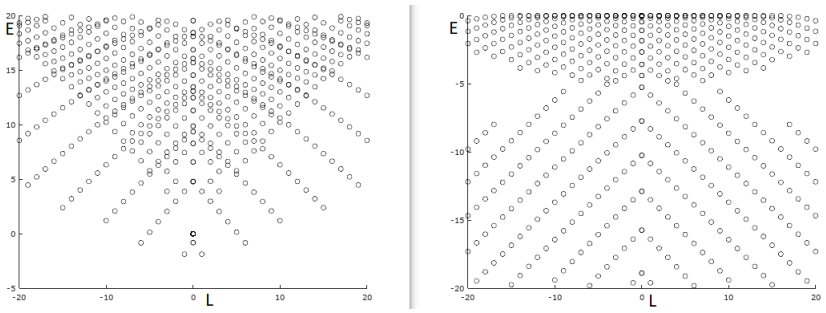



Figure 3.3: Inverted champagne bottle for $\theta = 0.1$.

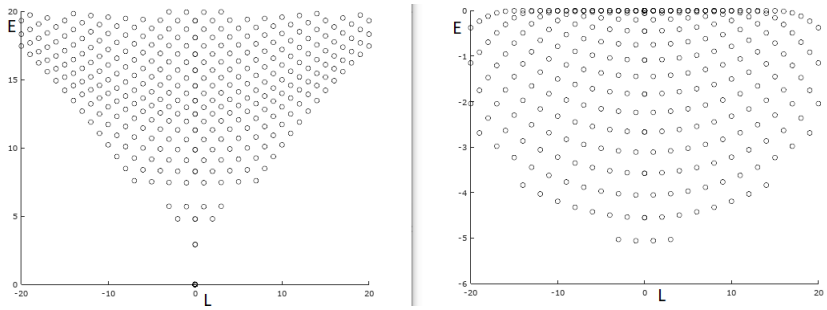



Figure 3.4: Inverted champagne bottle for $\theta = 0.5$.

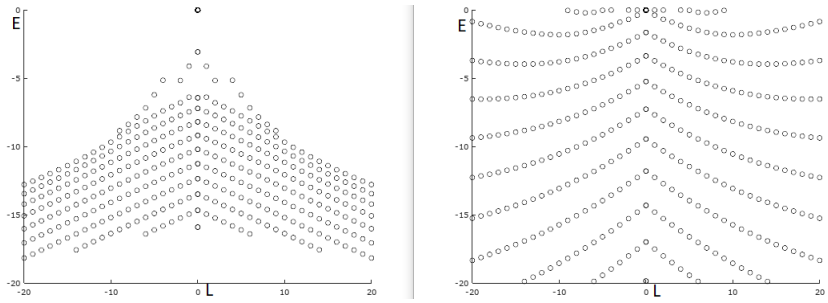



Figure 3.5: Inverted champagne bottle for $\theta = 1$.

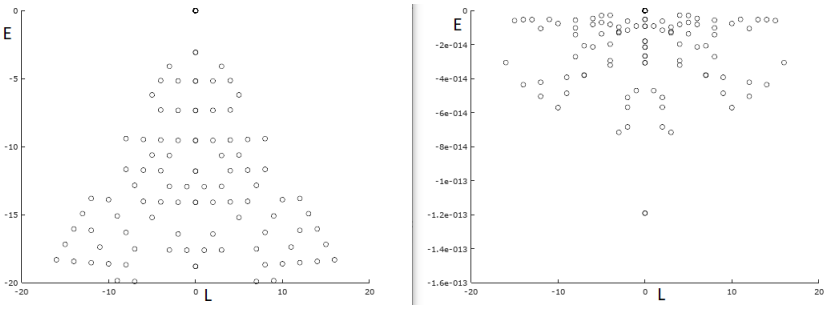



Figure 3.6: Inverted champagne bottle for $\theta = 1.5$.

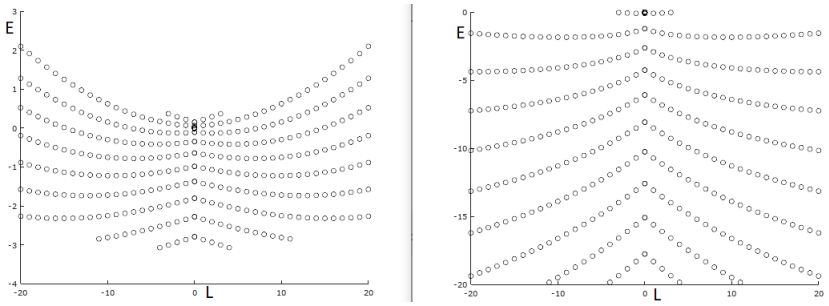



Figure 3.7: Inverted champagne bottle for $\theta = 0.87$.

# Conclusion

In this thesis, we have considered both classical and quantum monodromy in the champagne bottle potential. In both cases, we have seen the same pattern: A change in topology leads to monodromy. A consequence of the monodromy is the absence of a global structure. In the classical case, this was global action-angle variables, while in the quantum system, this corresponded to the absence of a global grid structure.

We have determined the quantum mechanical spectrum in two different ways: using semi-classical quantisation, and by expansion in the harmonic oscillator basis. Both methods were implemented in Octave, and the code is given in the appendix. These two methods were in close agreement with each other.

Using complex scaling, we have calculated the resonance spectrum of the upside-down champagne bottle potential. We argued that there should be some form of monodromy in this spectrum, but our method was unable to confirm this, due to strong dependence of the spectrum on the complex scaling parameter $\theta$.

As a suggestion for further research, one could try to adapt this method to other potentials in which we know quantum monodromy exists, such as the spherical pendulum. It is also possible to investigate monodromy in the upside-down champagne bottle by using semi-classical arguments. This would involve solving a tunnelling integral numerically.

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# Appendices

# Appendix A

# Numerical Algorithms

```
%For fixed l, compute the 2t matrix element
function [I] = t2inner(m,n,l)
if m == n
I = n+1;
elseif m == n+2
I = (1/2) * sqrt((n+2)^2 - l^2);
elseif m == n-2
I = (1/2) * sqrt(n^2 - l^2);
else
I = 0;
end
end
```

```
%For fixed l, compute the r^2 matrix element
function [I] = r2inner(m,n,l)
if m == n
I = n+1;
elseif m == n+2
I = (-1/2) * sqrt((n+2)^2 - l^2);
elseif m == n-2
I = (-1/2) * sqrt(n^2 - l^2);
else
I = 0;
end
end
```

```
%For fixed l, compute the r^4 matrix element
function [I] = r4inner(m,n,l)
if m==n-4
I= (1/4) * sqrt(n^2 - l^2) * sqrt((n-2)^2 - l^2);
```

```
5           elseif m==n-2
6           I = (n+1) * (-1/2) * sqrt(n^2 - l^2) + (-1/2) * sqrt(n^2
              - l^2) * (n-1);
7           elseif m ==n
8           I = (1/4) * ((n+2)^2 - l^2)  + (n+1)^2 + (1/4) * (n^2 - l
              ^2);
9           elseif m == n+2
10          I = (-1/2) * sqrt((n+2)^2 - l^2) * (n+3) + (n+1) * (-1/2)
               * sqrt((n+2)^2 - l^2);
11          elseif m == n+4
12          I = (1/4) * sqrt((n+2)^2 - l^2) * sqrt((n+4)^2 - l^2);
13          else
14          I = 0;
15          end
16          end
```

```
1           %Determining the spectrum of the champagne bottle
              hamiltonian
2           %depending on the parameter beta
3           clear all
4           close all
5
6           beta = 0.005;
7
8           %Computing the required matrix elements.
9           matSize = 100;
10          for l = 0:10
11          W = buildMat(l,beta,matSize);
12          eigVal = eig(W);
13          x = zeros(length(eigVal),1);
14          for i = 1:length(x)
15          x(i) = l;
16          end
17          plot(x,eigVal,'+k')
18          hold on
19          plot(-x,eigVal,'+k')
20          eigMat(l+1,:) = eigVal;
21
22          end
```

```
1           function [epsAr] = spectrumRootFinding(beta,nMin,nMax,
              lMin,lMax)
```

```
%Find the spectrum of the champagne bottle by
    semiclassical quantisation
p = nMax-nMin + 1;
q = lMax - lMin + 1;

for i = 1:q
l = lMin + i - 1;
n = nMin;
rhs = (n - 0.5) * pi;
F = @(E) quadrature(E,beta,l) - rhs;

Emin = -20;
D = discr([-2*beta 1 2*Emin -l^2]);
while D < 0
Emin = Emin + 1;
D = discr([-2*beta 1 2*Emin -l^2]);
end

Emax = 20;
fVal = F(Emax);
while fVal < 0
Emax = Emax + 1;
fVal = F(Emax);
end

epsAr(i,1) = bisection(F,Emin,Emax,10^-4,100);

for j = 2:p
n = nMin + j - 1;
rhs = (n - 0.5) * pi;
F = @(E) quadrature(E,beta,l) - rhs;
Emin = epsAr(i,j-1);
Emax = Emin + 5;
epsAr(i,j) = bisection(F,Emin,Emax,10^-4,100);
end
end
end
```

```
function [I]=quadrature(epsilon,beta,l)

p = [-2 * beta 1 2*epsilon -l^2];
q = roots(p);
q = sort(q);
```

```
6
7           zMin = q(2);
8           zMax = q(3);
9
10          fun = @(z) 1./(2*z) * sqrt(-2*beta*z.^3 + z.^2 + 2*
                epsilon.*z - 1.^2);
11
12          I = real(quad(fun,zMin,zMax,10^-6));
13          end
```

```
1  function [I]=quadrature(epsilon,beta,l)
2
3  p = [-2 * beta 1 2*epsilon -l^2];
4  q = roots(p);
5  q = sort(q);
6
7  zMin = q(2);
8  zMax = q(3);
9
10 fun = @(z) 1./(2*z) * sqrt(-2*beta*z.^3 + z.^2 + 2*epsilon.*z - l
       .^2);
11
12 I = real(quad(fun,zMin,zMax,10^-6));
13 end
```

```
1  #find the discriminant of a third order polynomial
2  function [Delta] = discr(p)
3
4  if length(p) == 4
5  a = p(1);
6  b = p(2);
7  c = p(3);
8  d = p(4);
9  Delta = 18*a*b*c*d - 4*b^3 * d + b^2 * c^2 - 4*a*c^3 - 27*a^2 * d
       ^2;
10 else
11 Delta = 0;
12 end
13 end
```

```
1  %Computes all matrix elements for H = t - 1/2 r^2 + beta * r^4
2
3  function [W] = buildMat(l,beta,matSize)
```

```
W = zeros(matSize);
for i = 1:matSize
for j = 1:matSize
n = 2*i + l - 2;
m = 2*j + l - 2;
W(i,j) = (1/2) * t2inner(n,m,l) + (-1/2) * r2inner(n,m,l) - beta
    * r4inner(n,m,l);
end
end
end
```

```
%Bisection method for rootfinding

function [root] = bisection(f,a,b,tol,maxIt)

left = f(a);
right = f(b);
if left*right > 0
break
end
N = 1;
while N < maxIt
c = (a+b)/2;
middle = f(c);
if (middle == 0 | (b-a)/2 < tol)
root = c;
break
end
N = N+1;
if middle * left > 0
a = c;
else
b = c;
end
end
break
end
```

```
%Analog to buildMat for the complex sccaling.
function [W] = complexBuildMat(l,beta,theta,matSize)
W = zeros(matSize);
for ii = 1:matSize
for jj = 1:matSize
```

```
n = 2*ii + l - 2;
m = 2*jj + l - 2;
W(ii,jj) = (1/2) * exp(-2*i*theta) * t2inner(n,m,l) + 1/2 * exp(2
    * i * theta) * r2inner(n,m,l) - beta * exp(4*i*theta) *
   r4inner(n,m,l);
end
end
end
```

```
clear all
close all

beta = 0.005;
theta = 0.87;
%Compute the complex scaling spectrum for the inverted champagne
   bottle

%Computing the required matrix elements.
matSize = 50;
L = 20;
for l = 0:L
W = complexBuildMat(l,beta,theta,matSize);
eigVals = eig(W);
eigMat(:,l+1) = eigVals;
end

M = matSize * (L + 1);
x = zeros(M,1);
y = zeros(M,1);

alpha = 1;
for ii = 1:L+1
for jj = 1:matSize
%     x(alpha) = ii-1;
%     y(alpha) = eigMat(jj,ii);
%     alpha = alpha + 1;
if imag(eigMat(jj,ii))<0 && imag(eigMat(jj,ii)) > -20 && abs(real
   (eigMat(jj,ii))) < 20
x(alpha) = ii-1;
y(alpha) = eigMat(jj,ii);
alpha = alpha + 1;
end
end
```

```
33 end
34
35 %Real Part
36 yr = real(y);
37 figure
38 scatter(x,yr,'k');
39 hold on
40 scatter(-x,yr,'k');
41 hold off
42
43 %Imaginary Part
44 yi = imag(y);
45 figure
46 scatter(x,yi,'k')
47 hold on
48 scatter(-x,yi,'k')
49 hold off
```