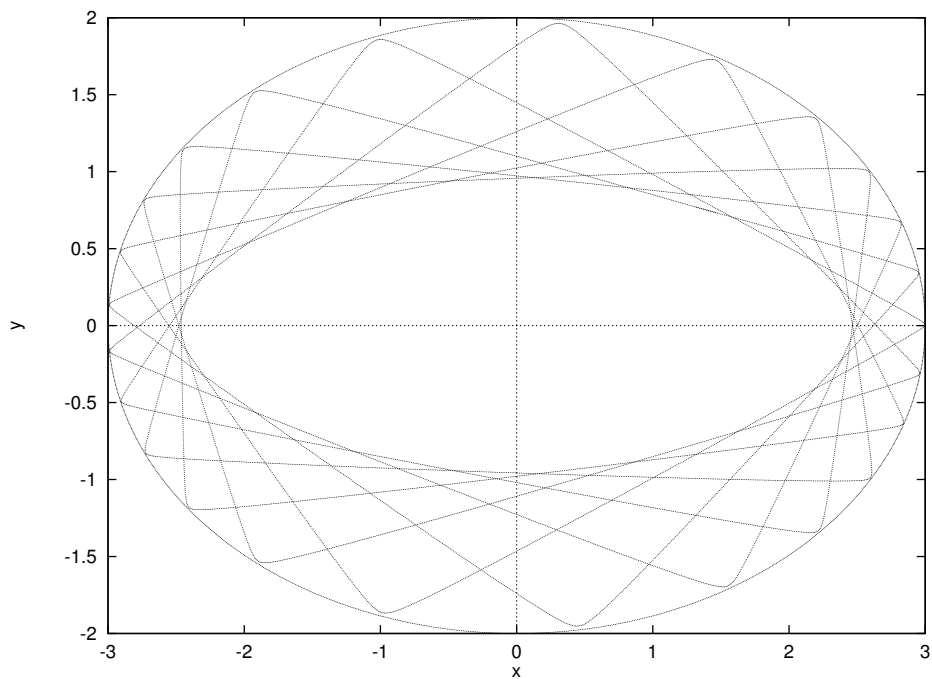


The Elliptical Billiard

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Introduction

At the present time, one might consider non-relativistic quantum mechanics as a mature and understood theory, on which not much research needs to be done. However, about two decades ago, a question was put forward that is still open: what is the equivalent of chaos in quantum mechanics?

For several decades it is known that classical mechanics can produce strange behavior, and that this behavior is generic in Hamilton-systems, rather than the behavior of regular mechanical systems that are traditionally covered by mechanics. *Chaos* can be observed everywhere in nature, mainly in the form of unpredictability: there always exists a time t_2 for which the state of the system cannot be predicted, even if the state were given with arbitrary high precision at time t_1 . This is caused by the exponential growth of small perturbations, which occurs only if the differential equations governing the system contain *non-linear terms*. This is called *sensitive dependence on initial conditions*.

Let's look at quantum mechanics now. There always exists some uncertainty in quantum mechanics, since it only makes predictions about chances. However, the *Schrödinger equation*, which governs non-relativistic quantum mechanics, is *linear* in the wave function Ψ , so there is no exponential growth of errors: no chaos in the above sense exists in quantum mechanics. But, since quantum mechanics is believed to be more fundamental than classical mechanics – which is supposed to be some limit of it – how can we explain that there is actually chaos on a macroscopic level?

To resolve this, one has to look more carefully to what chaos means on a quantum-mechanical level. Much research is done on this topic (Casati and Chirikov[7]), without a final answer as yet, though several suggestions have been made. Usually, one looks at a system which is known to be chaotic in the classical description, and one performs tests on the energy-levels, which should have certain characteristics. Those characteristics have never been properly founded on the fact that the classical system is chaotic. Therefore, it might be worth looking at the problem from a different viewpoint. I take a system which is not chaotic classically, and look at the statistics of the spectrum to see whether they possibly look anything like those of chaotic systems. If they do, then the usual link between classical chaos and quantum chaos would be wrong. The system that I will look at is the *elliptical billiard*: a free particle in two dimensions trapped in a box of which the edge has the shape of an ellipse. There is an article by Ayant and Arvieu[1] in which results are shown that indicate chaotic behavior, though the authors make no remarks about that. Also, this system has several difficulties in its quantum-mechanical version above those in the classical version which give hope for such a possibility.

In this thesis, the classical version of the billiard and its difficulties are treated first. A numerical simulation is used to illustrate the results. In the second part the quantum-mechanical version is discussed, as well as some theory regarding signs of chaos in quantum mechanics. Two approximation methods are used to calculate spectra, again numerically. In the third part, general two dimensional separable systems are considered. The elliptic billiard is included in that class. The similarities of these systems are shown. Finally, the results

of the investigations of these parts are summarized in the conclusion. Some details and theory follow in the appendices.

Acknowledgement

I'd like to express my thanks to prof. dr. Th. W. Ruijgrok for his assistance in my attempts to solve this problem and for the discussions we had, in some of which also prof. dr. N.G. van Kampen took part. I'd like to thank them for their critical attitude, which helped me distinguish more clearly rigorous facts from intuitive but sometimes false insights. I would also like to thank prof J. José for his encouragement, in what appeared to be the final stage of my thesis, to look at the $\bar{\Delta}_3$ -statistics, to provide a more complete picture. Finally, I'd like to thank my fellow students for the discussions and for their patience to listen to me.

1 Classical Part

In this part I will treat the classical elliptical billiard. First some analytical results are obtained, then some computer simulations are shown to illustrate and confirm these results. I'll conclude this part with a summary.

1.1 Theoretical Results

1.1.1 Two Constants of Motion

I have the following problem: consider a system of one particle with mass m moving within a billiard in the form of an ellipse – which means that it is allowed to move freely until it hits the boundary, from which it bounces back elastically. The ellipse has a long axis $2a$ and a short axis $2b$. The distance between the focal points is $2f$. a, b and f are related through $a^2 = b^2 + f^2$. It turns out, as is well known (Berry[4], Zhang, Merchant and Rae[25]), that this system has *two constants of motion*:

1. the energy E ,
2. the product \mathcal{L}^2 of the angular momentum l_1 with respect to one focal point and the angular momentum l_2 with respect to the other focal point.

Proofs that this last quantity is indeed a constant of motion are numerous, but sometimes too complicated [25]. One can actually see that \mathcal{L}^2 is a constant of motion as follows. I know that a ray from one focal point $(-f, 0)$ will bounce in the ellipse to the other focal point $(f, 0)$ as in figure 1, since a light ray follows a

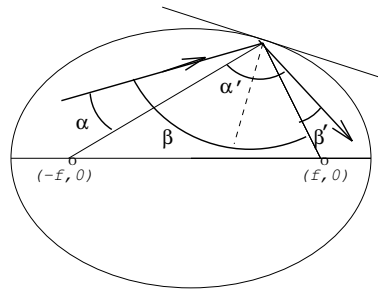


Figure 1: Collisions inside the ellipse

path of shortest length (Fermat's principle) and paths that encounter the edge, starting at one focal point and ending at the other all have the same length (by definition). Then all such paths are ordinary collisions with the edge, for which angle of incidence equals angle of reflection.

Now I turn to figure 1, in which the lines with arrows show a general collision. At the collision points, the angular momenta with respect to the focal point are given by the perpendicular distance to the lines connecting the collision point to the focal points and are thus proportion to $\sin \alpha$ and $\sin \beta$ respectively, and their product \mathcal{L}^2 is proportion to $\sin \alpha \sin \beta$. After the collision \mathcal{L}^2 therefore equals $\sin \alpha' \sin \beta'$ times the same proportionality-constant: the proportionality

constant depends on the product of the distances to the focal points, the square of the velocity and the mass, all of which do not change during the collision. Since the angles of incidence are equal to those of reflection, one sees from figure 1 that $\beta' = \alpha$ and $\alpha' = \beta$. So $\sin \alpha' \sin \beta' = \sin \alpha \sin \beta$ and thus \mathcal{L}^2 is conserved.

One would expect that this is all there is to this problem, since two constants of motion are in principle enough to solve the problem (in most cases). What the problem in this case is, will be stated in section 1.1.3, but it will require a more concrete formulation of the problem.

1.1.2 Elliptic Coordinates

The Hamiltonian describing the system has the form $\mathcal{H} = T + V$, where T is the standard kinetic energy term and V is a potential which is zero inside the ellipse and infinite outside of the ellipse. The ellipse is best implemented by a transformation to *elliptic coordinates*:

$$\begin{aligned} x &= f \cosh z \cos \theta \\ y &= f \sinh z \sin \theta \end{aligned} \quad (1.1)$$

Here, lines of constant z correspond to ellipses with foci at $(-f, 0)$ and $(f, 0)$, and an eccentricity of $1/\cosh z$; lines of constant θ correspond to hyperbola. Some special lines are:

- $\theta = 0$ — positive x -axis from $1 : [1, \infty[$
- $\theta = \pi$ — negative x -axis from $-1 :]-\infty, -1]$
- $z = 0$ — interval on the x -axis : $[-1, 1]$
- $z = z_b$ — an ellipse.

The ellipse $z = z_b$ will be the elliptical wall in my problem, so $V(z, \theta)$ will be zero for $z < z_b$ and infinite for $z > z_b$. Note that $a = f \cosh z_b$ and $b = f \sinh z_b$.

Now I will calculate the form the Hamiltonian \mathcal{H} takes when the coordinate transformation to elliptic coordinates is applied. I will use the Lagrangian, as in appendix A.1. The Lagrangian in my problem is

$$L(x, y, \dot{x}, \dot{y}) = \frac{m}{2}(\dot{x}^2 + \dot{y}^2) - V(x, y) \quad (1.2)$$

Using the equation (1.1) and the chain-rule to obtain expressions for \dot{x} and \dot{y} in terms of \dot{z} and $\dot{\theta}$:

$$\begin{aligned} \dot{x} &= f \sinh z \cos \theta \dot{z} - f \cosh z \sin \theta \dot{\theta} \\ \dot{y} &= f \cosh z \sin \theta \dot{z} + f \sinh z \cos \theta \dot{\theta} \end{aligned} \quad (1.3)$$

I can rewrite the Lagrangian in terms of these as

$$L(z, \theta, \dot{z}, \dot{\theta}) = \frac{mf^2}{2}M(z, \theta)(\dot{z}^2 + \dot{\theta}^2) - V(x(z, \theta), y(z, \theta)) \quad (1.4)$$

where $M(z, \theta)$ is a function that will turn up in many expressions. It is defined as

$$M(z, \theta) = \cosh^2 z - \cos^2 \theta \quad (1.5)$$

From the form (1.4) I compute the generalized momenta, finding

$$\begin{aligned} \dot{z} &= \frac{p_z}{mf^2 M(z, \theta)} \\ \dot{\theta} &= \frac{p_\theta}{mf^2 M(z, \theta)} \end{aligned} \quad (1.6)$$

With these expressions the Hamiltonian can be derived using equation (A.2). I found that

$$\mathcal{H} = \frac{p_z^2 + p_\theta^2}{2mf^2 M(z, \theta)} + V(z, \theta) \quad (1.7)$$

in which I denoted $V(x(z, \theta), y(z, \theta))$ simply by $V(z, \theta)$. I also need the expression for \mathcal{L}^2 in terms of elliptic coordinates. By definition,

$$\begin{aligned} l_1 &= (x - f)p_y - yp_x \\ l_2 &= (x + f)p_y - yp_x \end{aligned} \quad (1.8)$$

Using that $p_x = m\dot{x}$ and $p_y = m\dot{y}$ and (1.3) I find for l_1 and l_2 :

$$\begin{aligned} l_1 &= \frac{p_\theta \sinh z - p_z \sin \theta}{\cosh z + \cos \theta} \\ l_2 &= \frac{p_\theta \sinh z + p_z \sin \theta}{\cosh z - \cos \theta} \end{aligned} \quad (1.9)$$

Thus $\mathcal{L}^2 = l_1 l_2$ is given by

$$\mathcal{L}^2 = \frac{\sinh^2 z p_\theta^2 - \sin^2 \theta p_z^2}{M(z, \theta)} \quad (1.10)$$

1.1.3 Poisson-bracket Crisis

A commonly known characteristic of a constant of motion A is that the Poisson-brackets with the Hamiltonian, $\{\mathcal{H}, A\}$ vanish (appendix A.1). Since \mathcal{L}^2 is conserved, I tried to calculate $\{\mathcal{H}, \mathcal{L}^2\}$ using definition (A.4). This task is divided in two, namely calculating $\{T, \mathcal{L}^2\}$ and calculating $\{V, \mathcal{L}^2\}$. The calculation of $\{T, \mathcal{L}^2\}$ is easiest in plain Cartesian coordinates. Since T does not depend on x or y , only two terms remain to be calculated:

$$\{T, \mathcal{L}^2\} = -\frac{p_x}{m} \frac{\partial \mathcal{L}^2}{\partial x} - \frac{p_y}{m} \frac{\partial \mathcal{L}^2}{\partial y}$$

It is easy to see that $\frac{\partial l_1}{\partial x} = \frac{\partial l_2}{\partial x} = p_y$ and $\frac{\partial l_1}{\partial y} = \frac{\partial l_2}{\partial y} = -p_x$, so that this becomes:

$$\begin{aligned} \{T, \mathcal{L}^2\} &= -\frac{p_x}{m} [p_y l_2 + p_y l_1] - \frac{p_y}{m} [-p_x l_2 - p_x l_1] \\ &= 0 \end{aligned} \quad (1.11)$$

This result is hardly surprising since all angular momenta of a free particle¹ are conserved. In elliptic coordinates it would be more elaborate to get this result.

Now I will calculate $\{V, \mathcal{L}^2\}$. Using \mathcal{L}^2 from (1.10) it follows that

$$\begin{aligned} \{V, \mathcal{L}^2\} &= \frac{\partial \mathcal{L}^2}{\partial p_z} \frac{\partial V}{\partial z} + \frac{\partial \mathcal{L}^2}{\partial p_\theta} \frac{\partial V}{\partial \theta} \\ &= \frac{-2 \sin^2 \theta}{M(z, \theta)} p_z \frac{\partial V}{\partial z} + \frac{2 \sinh^2 z}{M(z, \theta)} p_\theta \frac{\partial V}{\partial \theta} \end{aligned}$$

Thus

$$\begin{aligned} \{\mathcal{H}, \mathcal{L}^2\} &= \{V, \mathcal{L}^2\} \\ &= 2mf^2 \left[\sinh^2 z \dot{\theta} \frac{\partial V}{\partial \theta} - \sin^2 \theta \dot{z} \frac{\partial V}{\partial z} \right] \end{aligned} \quad (1.12)$$

Now V may be zero in the interior of the ellipse, its derivative certainly cannot be considered zero: it is rather infinite at the boundary. This is what gave rise to a further investigation on this problem even in the classical case. I may add that in the quantum case a similar problem arises for the commutator of \mathcal{H} and the quantum version of \mathcal{L}^2 . Just as the angular momentum is conserved in a circular potential, one might wonder if \mathcal{L}^2 can be conserved for an elliptical potential $V(z)$. This is not the case. For such a potential

$$\frac{d\mathcal{L}^2}{dt} = 2mf^2 \sin^2 \theta \dot{z} \frac{dV}{dz}$$

where the derivative to z is now a total derivative. V does not depend on the momenta nor on time, so

$$\dot{z} \frac{dV}{dz} = \frac{dV}{dt}$$

for any trajectory. If this system has to be close to a billiard-system, V has to be practically zero (or constant) in some region inside the ellipse – the *free region* – and non-zero in an area closer to the edge – the *interaction region*². Consider a trajectory beginning and ending in the free region at t_0, t_1 respectively. Since $V = 0$ there, the kinetic energy is the same at t_0 and t_1 . \mathcal{L}^2 has changed by an amount

$$\begin{aligned} \Delta \mathcal{L}^2 &= \int_{t_0}^{t_1} \frac{d\mathcal{L}^2}{dt} dt = 2mf^2 \int_{t_0}^{t_1} \sin^2 \theta \frac{dV}{dt} dt \\ &= \left[2mf^2 \sin^2 \theta V \right]_{t_0}^{t_1} - 2mf^2 \int_{t_0}^{t_1} \sin 2\theta V \dot{\theta} dt \\ &= -2mf^2 \int_{t_0}^{t_1} \sin 2\theta(t) V(z(t)) d\theta(t) \end{aligned} \quad (1.13)$$

for this trajectory $(z(t), \theta(t))$. Note that \mathcal{L}^2 is conserved for a free particle. I now look at the following case that $V(z)$ gives an approximation of the step-function,

¹in which case \mathcal{H} is just T

²in most cases, there is some arbitrariness in the boundary between these regions.

so $\frac{dV}{dz} \geq 0$. In section 1.2.1, I will see that there exist trajectories for which $\sin 2\theta$ does not change sign and for which z can be regarded as a single valued function of θ . These are trajectories that look like ordinary collisions with a wall, taking place in one quadrant, so on physical ground these trajectories have to exist if V is to give a good approximation of a billiard. Then the integral becomes just an integral over θ from θ_0 to θ_1 . For these kinds of trajectories, which go through the interaction region, the following holds:

$$\int_{\theta_0}^{\theta_1} V(z(\theta)) d\theta = \Omega > 0$$

Since they lie totally in one quadrant, I have

$$\min_{(\theta_0, \theta_1)} |\sin 2\theta_i| = \sigma > 0$$

Therefore, I can get

$$\begin{aligned} |\Delta \mathcal{L}^2| &= 2mf^2 \int_{\theta_0}^{\theta_1} |\sin 2\theta| V(z(\theta)) d\theta \\ &\geq 2mf^2 \sigma \int_{\theta_0}^{\theta_1} V(z(\theta)) d\theta \\ &= 2mf^2 \sigma \Omega \end{aligned} \tag{1.14}$$

This lower bound for $|\Delta \mathcal{L}^2|$ is larger than zero for these trajectories, so \mathcal{L}^2 is not conserved. The restriction to collisions inside some quadrant was really necessary since on symmetry grounds one sees that for a trajectory that reaches its maximum z value at $\theta = \pi/2$ (or $0, \pi, 3\pi/2$), the kernel of integral is odd in θ , so \mathcal{L}^2 is conserved. \mathcal{L}^2 is also conserved for trajectories in which $\theta_0 = \theta_1$ (which were implicitly excluded by (1.14). Such trajectories are the periodic solution $[(-a, 0), (a, 0)]$ and $[(0, -b), (0, b)]$. The largest values for $|\Delta \mathcal{L}^2|$ can be expected when σ and Ω are large. Ω is large if the intersection of the trajectory with the interaction region is large, which happens when the velocity at t_0 is nearly parallel to the ellipse. This will be confirmed by the computer simulations in section 1.2.1.

1.1.4 Conserved Generalizations of \mathcal{L}^2

In this section I will give a general conserved quantity besides the energy for a fairly large class of potentials. The construction I will give here is not the original one that led me to this constant of motion, in which I used the Hamilton-Jacobi formalism and searched for separable systems. This demand could be fulfilled by special forms of the potential from the same class as I will find using the following construction.

First, I will have to make the following Ansatz. I know that \mathcal{L}^2 behaves almost as a conserved quantity, and that the deviations from that are – for potentials that approximate the hard wall – local: they originate from the interaction region. I try to fix the non-conservative behavior by adding a term which depends only on the coordinates:

$$Z = \mathcal{L}^2 + X(z, \theta) \tag{1.15}$$

and I demand that

$$\dot{Z} = 0 \quad (1.16)$$

Using the equations of motion (\mathcal{H} is given in (1.7)):

$$\begin{aligned} \dot{p}_z &= T \frac{\sinh 2z}{M(z, \theta)} - \frac{\partial V}{\partial z} \\ \dot{p}_\theta &= T \frac{\sin 2\theta}{M(z, \theta)} - \frac{\partial V}{\partial \theta} \end{aligned} \quad (1.17)$$

and \dot{z} and $\dot{\theta}$ given by (1.6), I find

$$\dot{\mathcal{L}}^2 = \frac{2}{M(z, \theta)} [p_z \sin^2 \theta \frac{\partial V}{\partial z} - p_\theta \sinh^2 z \frac{\partial V}{\partial \theta}] \quad (1.18)$$

$$\dot{X} = \frac{1}{mf^2 M(z, \theta)} [p_z \frac{\partial X}{\partial z} + p_\theta \frac{\partial X}{\partial \theta}] \quad (1.19)$$

so (1.16) becomes³

$$\begin{aligned} -2mf^2 \sin^2 \theta \frac{\partial V}{\partial z} &= \frac{\partial X}{\partial z} \\ 2mf^2 \sinh^2 z \frac{\partial V}{\partial \theta} &= \frac{\partial X}{\partial \theta} \end{aligned} \quad (1.20)$$

Now if X is well-behaved, I have

$$\frac{\partial^2 X}{\partial z \partial \theta} = \frac{\partial^2 X}{\partial \theta \partial z} \quad (1.21)$$

so that

$$\begin{aligned} 0 &= \frac{\partial}{\partial \theta} \left[\sin^2 \theta \frac{\partial V}{\partial z} \right] + \frac{\partial}{\partial z} \left[\sinh^2 z \frac{\partial V}{\partial \theta} \right] \\ &= 2 \sin \theta \cos \theta \frac{\partial V}{\partial z} + 2 \sinh z \cosh z \frac{\partial V}{\partial \theta} + (\sin^2 \theta + \sinh^2 z) \frac{\partial^2 V}{\partial z \partial \theta} \end{aligned}$$

If I write

$$V(z, \theta) = W(z, \theta)/M(z, \theta) \quad (1.22)$$

then this becomes

$$\frac{\partial^2 V}{\partial \theta \partial z} = \frac{1}{M(z, \theta)} \left[-\frac{\frac{\partial W}{\partial z}}{M(z, \theta)} \frac{\partial M}{\partial \theta} - \frac{\frac{\partial W}{\partial \theta}}{M(z, \theta)} \frac{\partial M}{\partial z} + 2 \frac{W(z, \theta)}{M^2(z, \theta)} \frac{\partial M}{\partial z} \frac{\partial M}{\partial \theta} \right] \quad (1.23)$$

From (1.22) I can also calculate

$$\frac{\partial^2 V}{\partial \theta \partial z} = \frac{1}{M(z, \theta)} \left[\frac{\partial^2 W}{\partial \theta \partial z} - \frac{\frac{\partial W}{\partial z}}{M(z, \theta)} \frac{\partial M}{\partial \theta} - \frac{\frac{\partial W}{\partial \theta}}{M(z, \theta)} \frac{\partial M}{\partial z} + 2 \frac{W(z, \theta)}{M^2(z, \theta)} \frac{\partial M}{\partial z} \frac{\partial M}{\partial \theta} \right] \quad (1.24)$$

³I split the p_θ and the p_z parts, since (1.16) is to hold for all initial values.

So I conclude that

$$\frac{\partial^2 W}{\partial \theta \partial z} = 0 \Rightarrow W(z, \theta) = V_1(z) + V_2(\theta) \quad (1.25)$$

and V has to be of the form

$$V(z, \theta) = \frac{V_1(z) + V_2(\theta)}{M(z, \theta)} \quad (1.26)$$

Now (1.16) has a solution. From (1.20) one easily sees that

$$\begin{aligned} X &= -2mf^2 \sin^2 \theta V(z, \theta) + h(\theta) \\ X &= 2mf^2 \sinh^2 z V(z, \theta) + g(z) \end{aligned}$$

where h and g are still to be determined. Substituting (1.26) and some rearranging gives

$$\begin{aligned} X &= \frac{-2mf^2 \sin^2 \theta V_1(z)}{M(z, \theta)} + \frac{\sin^2 \theta [-2mf^2 V_2(\theta) + h(\theta)]}{M(z, \theta)} + \frac{\sinh^2 z h(\theta)}{M(z, \theta)} \\ X &= \frac{2mf^2 \sinh^2 z V_2(\theta)}{M(z, \theta)} + \frac{\sinh^2 z [2mf^2 V_1(z) + g(z)]}{M(z, \theta)} + \frac{\sin^2 \theta g(z)}{M(z, \theta)} \end{aligned}$$

Since (1.20) contains only derivatives, X can be determined from them only up to a constant. To keep a tight connection between Z and \mathcal{L}^2 , I set the constant to zero. Choosing h and g to be

$$\begin{aligned} h(\theta) &= 2mf^2 V_2(\theta) \\ g(z) &= -2mf^2 V_1(z) \end{aligned}$$

will cause the two expressions for X to be the same, namely

$$X(z, \theta) = 2mf^2 \frac{V_2(\theta) \sinh^2 z - V_1(z) \sin^2 \theta}{M(z, \theta)} \quad (1.27)$$

So now I have found a second constant of motion for systems with the special potential (1.26)⁴, expressed in elliptic coordinates, and I see that it reduces to \mathcal{L}^2 if V goes to zero, since X is proportional to V . In principle, that (1.26) can represent a potential is easily seen from the following argument. I look for potentials, such that X and V are not singular. In order to cope with the singularities at the focal points, V_1 and V_2 have to be of the form

$$\begin{aligned} V_1(z) &= \sinh^2 z v_1(z) \\ V_2(\theta) &= \sin^2 \theta v_2(\theta) \end{aligned} \quad (1.28)$$

Take for simplicity $v_2 = 0$. One can look at a limiting procedure in which V in each step has the form of (1.26), where in the limit v_1 will go to an infinite step function, being zero inside the ellipse and infinite outside of it. Then V itself will also be of that form, since inside it is $0/M(z, \theta) = 0$ and outside it

⁴which also renders the system separable in the Hamilton-Jacobi formalism.

is $\infty/M(z, \theta) = \infty$; V represents a hard wall. So one sees that it is possible to regard a hard wall potential as being of the form of (1.26). One also sees from the form of the second constant of motion how to avoid infinity in the Poisson-brackets: add a term which contains the potential and which will thus cancel the infinity, since it goes to infinity itself. Notice that the above is not possible for a potential depending on z only, since it does not have the required form. That the Poisson bracket is now indeed zero is proven in section 2.2.3 for both the classical case and the quantum case.

Another way of looking at this result is to say that the boundary is a kinematically prohibited area due to the conservation of energy, if one includes a infinite potential on and outside of the ellipse: a particle with finite energy cannot be there. Then (1.12) reduces to zero because V is zero inside the ellipse. From the expression (1.10) for \mathcal{L}^2 , it is not clear that the boundary is prohibited with respect to that second constant of motion. From the conservation of Z and its form according to (1.15) and (1.27), one sees that the boundary is again a Z -prohibited area: a particle with finite Z cannot be there. And Z reduces to \mathcal{L}^2 inside the ellipse. So both the conservation of \mathcal{L}^2 and the elliptical boundary are manifest in Z .

The following remark shows how the inclusion of a potential of the form (1.26), which can be seen as the manifestation of the boundary, changes various formulas. I already saw that T is replaced by $T + V$, \mathcal{L}^2 is replaced by $\mathcal{L}^2 + X$. All that happens on the level of formulas is the following substitution

$$\begin{aligned} p_z^2 &\rightarrow p_z^2 + 2mf^2V_1(z) \\ p_\theta^2 &\rightarrow p_\theta^2 + 2mf^2V_2(\theta) \end{aligned} \quad (1.29)$$

As I already mentioned, I should have a "separated problem" now. To what extent separation has been reached, I will show in the next section.

1.1.5 Nature of the Second Constant of Motion

In this section I will give some further results that I found regarding the second constant of motion Z . First I will derive some bounds for Z . To emphasize that Z and \mathcal{H} are constant, I denote their values by l and E respectively. The equalities

$$Z = 2mf^2 \sinh^2 z \mathcal{H} - p_z^2 - 2mf^2V_1 \quad (1.30)$$

and

$$-Z = 2mf^2 \sin^2 z \mathcal{H} - p_\theta^2 - 2mf^2V_2 \quad (1.31)$$

give me the estimates

$$\begin{aligned} l &\leq 2mf^2 \sinh^2 z_b = 2mb^2E \\ -l &\leq 2mf^2E \end{aligned}$$

or

$$-2mf^2E \leq l \leq 2mb^2E \quad (1.32)$$

These bounds also hold in the quantum-mechanical case. Notice that negative values for \mathcal{L}^2 correspond to paths that cross the x -axis between the focal points. When $V=0$ inside the ellipse, \mathcal{L}^2 takes its lowest value for the periodic orbit that runs up down along the y -axis between $(0, b)$ and $(0, -b)$. The largest value of \mathcal{L}^2 corresponds a path touching the ellipse, which exists only as a limiting case. I wondered how separated the problem would be, fixing the values of l and E . The expressions for l and E form a set of linear equations in $(p_\theta^2 + 2mf^2V_2)$ and $(p_z^2 + 2mf^2V_1)$. The solution is

$$\begin{aligned} p_z^2 &= -2mf^2V_1 - l \cosh^2 z + (l + 2mf^2E) \sinh^2 z \\ p_\theta^2 &= -2mf^2V_2 + l \cos^2 \theta + (l + 2mf^2E) \sin^2 \theta \end{aligned} \quad (1.33)$$

I see that p_z depends on z only, and p_θ depends on θ only⁵. However, this does not mean that the directions z and θ are totally decoupled, since I still have (1.6), where \dot{z} and $\dot{\theta}$ depend on both z and θ !

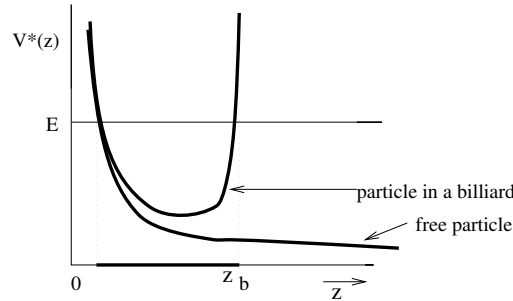


Figure 2: Bounds on a trajectory with $l > 0$

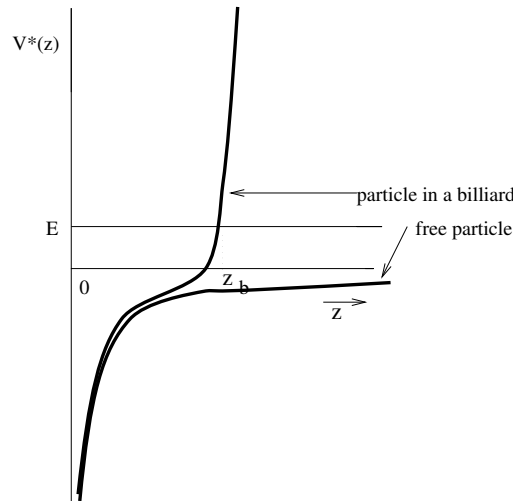


Figure 3: Bounds on a trajectory with $l < 0$

⁵which is not surprising since in my first derivation I used the Hamilton-Jacobi formalism to find separable systems.

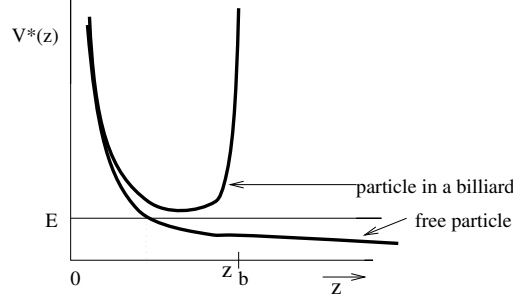


Figure 4: Bounds of prohibited orbits

I can, however, write down an equation for the path of the particle:

$$\frac{dz}{d\theta} = \frac{p_z}{p_\theta} \quad (1.34)$$

in which the M -terms cancel. The momenta are given as a function of z and θ in (1.33), so

$$\frac{dz}{d\theta} = \frac{p_z}{p_\theta} = \pm \frac{\sqrt{-2mf^2V_1 - l \cosh^2 z + (l + 2mf^2E) \sinh^2 z}}{\sqrt{-2mf^2V_2 + l \cos^2 \theta + (l + 2mf^2E) \sin^2 \theta}} \quad (1.35)$$

Separating variables, and integrating over a trajectory from (z_0, θ_0) to (z_1, θ_1) gives me

$$\begin{aligned} & \int_{z_0}^{z_1} \frac{dz}{\sqrt{-2mf^2V_1 - l \cosh^2 z + (l + 2mf^2E) \sinh^2 z}} \\ &= \pm \int_{\theta_0}^{\theta_1} \frac{d\theta}{\sqrt{-2mf^2V_2 + l \cos^2 \theta + (l + 2mf^2E) \sin^2 \theta}} \end{aligned}$$

If I call the primitive of $[-2mf^2V_1 - l \cosh^2 z + (l + 2mf^2E) \sinh^2 z]^{-\frac{1}{2}}$, $F(z)$, and that of $[-2mf^2V_2 + l \cos^2 \theta + (l + 2mf^2E) \sin^2 \theta]^{-\frac{1}{2}}$, $G(\theta)$:

$$\begin{aligned} F(z') &= \int^{z'} \frac{dz}{\sqrt{-2mf^2V_1 - l \cosh^2 z + (l + 2mf^2E) \sinh^2 z}} \\ G(\theta') &= \int^{\theta'} \frac{\pm d\theta}{\sqrt{-2mf^2V_2 + l \cos^2 \theta + (l + 2mf^2E) \sin^2 \theta}} \end{aligned} \quad (1.36)$$

I get

$$F(z_1) - F(z_0) = G(\theta_1) - G(\theta_0)$$

Since $\frac{dF}{dz}$ is non-zero if $F(z)$ exists, the inverse of F^{-1} , exists and the trajectory is

$$z(\theta) = F^{-1}(F(z_0) - G(\theta_0) + G(\theta)) \quad (1.37)$$

The primitives in (1.36) do not always exist⁶. Whether they exist or not depends on l/E , as I will show, and this determines the shape of the area to which the trajectory is confined. So I look at the implications of

$$\begin{aligned} -2mf^2V_1 - l \cosh^2 z + (l + 2mf^2E) \sinh^2 z &\geq 0 \\ -2mf^2V_2 + l \cos^2 \theta + (l + 2mf^2E) \sin^2 \theta &\geq 0 \end{aligned}$$

these can be rewritten as

$$E \geq V_z^*(z, l) = \frac{V_1(z) + \frac{l}{2mf^2}}{\cosh^2 z - 1} \quad (1.38)$$

$$E \geq V_\theta^*(\theta, l) = \frac{V_2(\theta) - \frac{l}{2mf^2}}{1 - \cos^2 \theta} \quad (1.39)$$

Now $\cosh^2 z \geq 1$ and $\cos^2 \theta \leq 1$, so these bounds are non-trivial only when

$$l + 2mf^2V_1(z) \geq 0 \quad (1.40)$$

$$l - 2mf^2V_2(\theta) \leq 0 \quad (1.41)$$

respectively. Thus when (1.40) holds, (1.38) applies and states that the trajectory is bound by ellipses. When (1.41) is fulfilled, (1.39) applies, stating that the trajectory is confined by hyperbola. When $V_1 = V_2 = 0$, the conditions (1.40) and (1.41) are mutually exclusive for non-zero l . For l negative, the motion is confined to an area including the y -axis, bounded by two hyperbola, otherwise it is bounded to the area outside of an ellipse. When a V_1 is added that looks like an infinite step function, the bounds to the motion are changed as follows. To find the bounds, I have to look for values of θ and z for which $V_z^*(z) = E$ and V_θ^* , which I will refer to as the roots of these equations. For trajectories that were bounded by an ellipse inside the billiard, I now gain a root, as is most easily seen graphically in figure 2, where I depicted V_z^* from (1.38). The new bound is at the edge of the billiard, as one would expect. The old bound is hardly effected by adding this potential. For trajectories with $l < 0$, equation (1.38), which had no roots before, also gets a root at the edge of the ellipse, as can be seen in figure 3. Finally, I look at what happens to trajectories that lay outside of the billiard. Again, this is done graphically, in figure 4. I see that the root they had disappears, and (1.40) is never fulfilled. Adding V_2 would change the character of the system, V no longer being zero in the interior of the billiard. I therefore did not consider this case.

1.2 Numerical Results

1.2.1 Computer Simulations

Investigating the properties of an elliptical billiard and the dependence on the form of an approximate potential as discussed in section 1.1.4, I conducted some computer-simulations, in which I could keep track of the constants of motion. The simulations were based on a discretization of time in Hamilton's equations

⁶They are not always real.

of motion (1.6) and (1.17). I performed all calculations in elliptic coordinates since the transformation $(x, y) \rightarrow (z, \theta)$ needed to be able to use potentials of the form (1.26), turned out to be numerically difficult. The computational method I used was a fourth-order non-adaptive Runge-Kutta method, described in appendix D.1. To apply the method I have to find the \vec{f} from D.1, which is according to (A.3)

$$\vec{f} = \left(\frac{\partial \mathcal{H}}{\partial p_z}, \frac{\partial \mathcal{H}}{\partial p_\theta}, -\frac{\partial \mathcal{H}}{\partial z}, -\frac{\partial \mathcal{H}}{\partial \theta} \right)$$

taking \vec{y} to be $(z, \theta, p_z, p_\theta)$. \mathcal{H} is given in (1.7), and its derivatives were already given in (1.6) and (1.17). For V I took two different forms, corresponding to the two cases also discussed in section 1.1.4:

- (I) the case that V depends only on z ,
- (II) the case that V is of the form (1.26).

For V and v_1 I will use functions that look like step functions and that depend on some parameters which control the steepness and the height of the potential wall. I used

$$\frac{V_0}{\eta} \left[\frac{1}{2} + \frac{1}{\pi} \arctan\left(\frac{z^2 - z_b^2}{\eta}\right) \right]$$

for V , v_1 respectively, where η controls the steepness, $\frac{V_0}{\eta}$ controls the height. If $\eta \rightarrow 0$, the function becomes the infinite step function needed for a perfect billiard. Notice that, calling V in case (I) V_I , in case (II) I have $V_{II} = \sinh^2 z V_I / (\sinh^2 z + \sin^2 \theta)$. So V_I and V_{II} are equal for $\sin \theta = 0$: the x -axis, but V_{II} is smaller than V_I for $\sin^2 \theta = 1$ (the y -axis), by a factor of $\sqrt{1 - \epsilon^2}$. To monitor the accuracy and see if \mathcal{L}^2 is conserved, I displayed a graph of E and \mathcal{L}^2 . Actually, to see the accuracy of E , I displayed $\frac{\Delta E}{E_0} = \frac{E - E_0}{E_0}$, where E_0 is the initial energy of the particle. I used a scale of some tenths of a percent, and I could not detect any deviation from zero in case (I), which means that

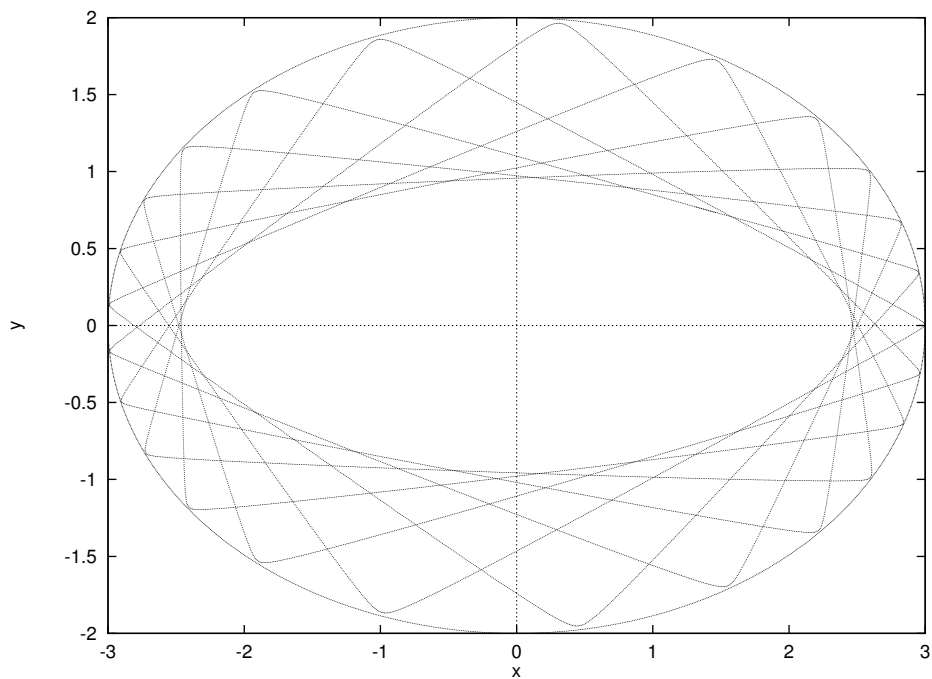
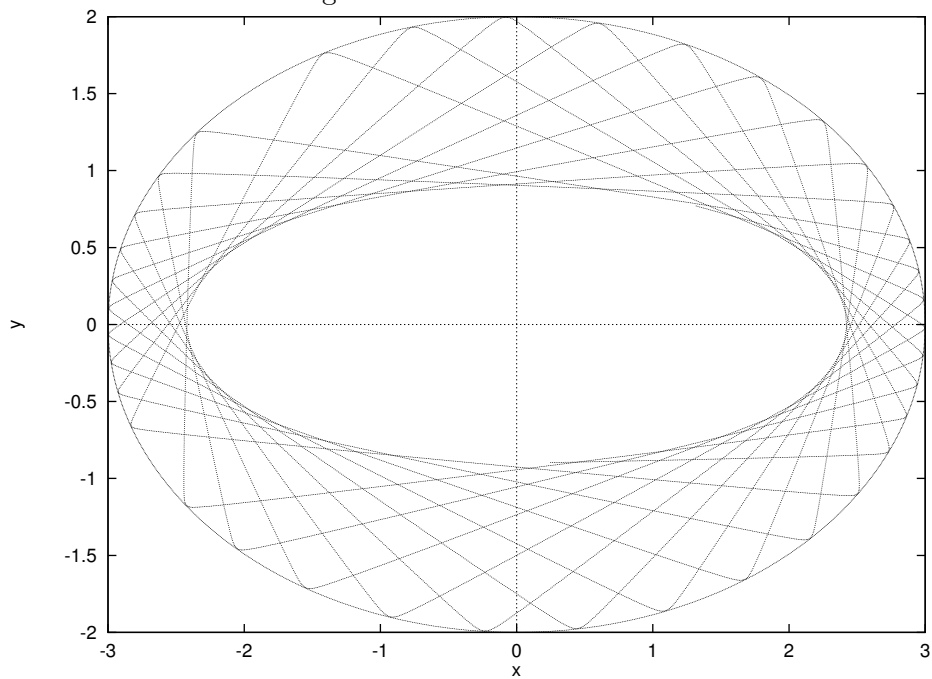
$$\frac{\Delta E}{E_0} < 2.5 \times 10^{-4} \quad (1.42)$$

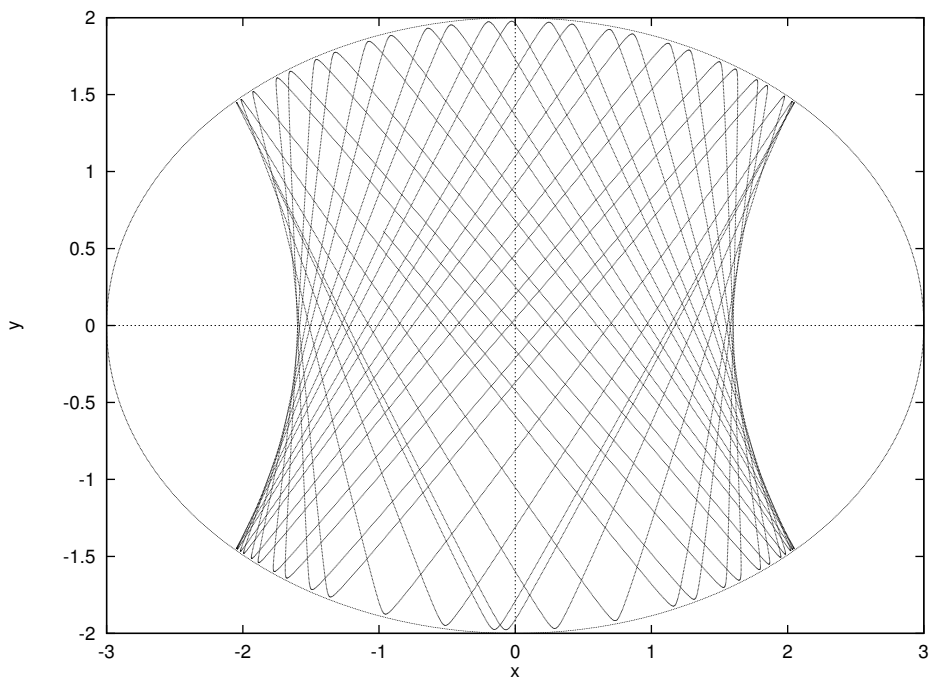
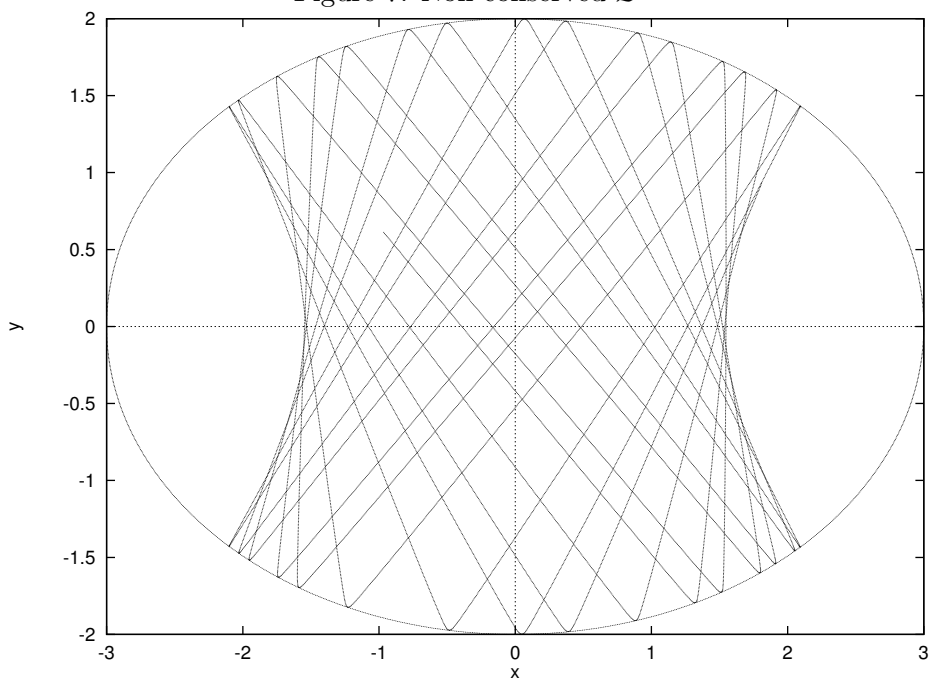
which is rather good, I think. In case (II), which required more calculations, the accuracy decreased to some percents, but the simulation still shows the qualitative aspects of a separable potential. The results are shown in figures 5 to 12, for the following values:

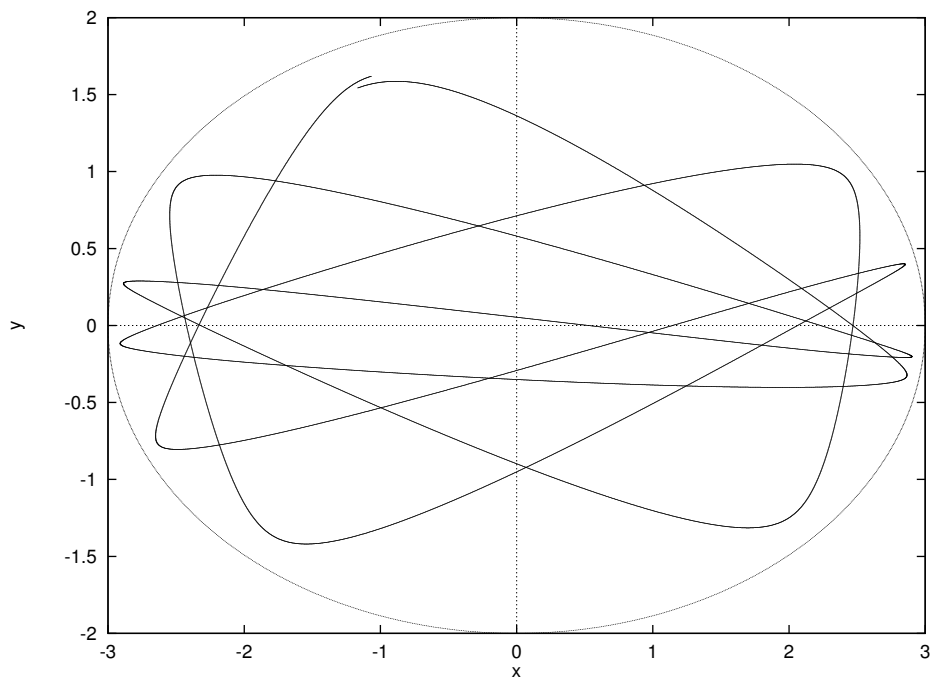
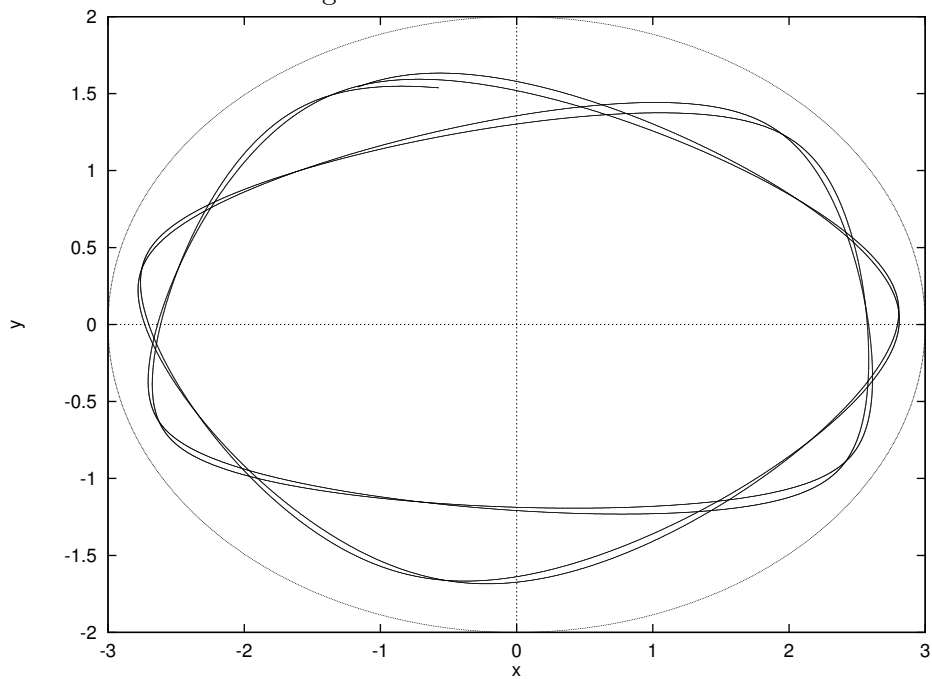
- 5, 6: $\eta=0.01$; $V_0 = 0.001$; $(z, \theta)_0 = (0.40, 1.00)$; $(p_z, p_\theta)_0 = (0, -0.7)$
- 7, 8: $\eta=0.01$; $V_0 = 0.001$; $(z, \theta)_0 = (0.30, 2.00)$; $(p_z, p_\theta)_0 = (-0.42, -0.3)$
- 9, 10: $\eta=0.01$; $V_0 = 0.001$; $(z, \theta)_0 = (0.70, 2.00)$; $(p_z, p_\theta)_0 = (0.01, -0.2)$
- 11, 12: $\eta=0.10$; $V_0 = 0.010$; $(z, \theta)_0 = (0.40, 1.00)$; $(p_z, p_\theta)_0 = (0, -0.15)$

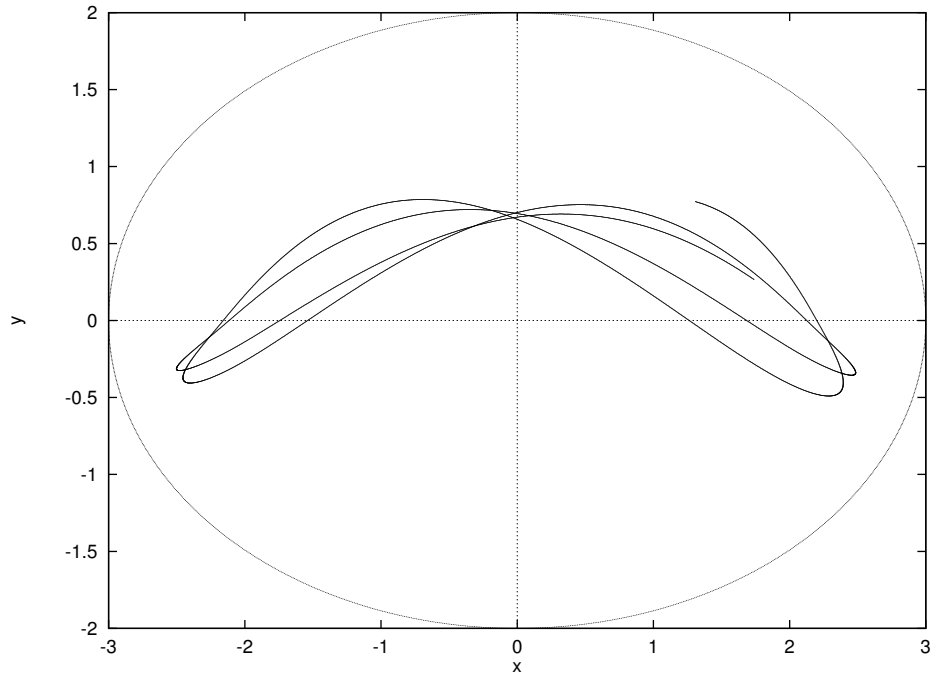
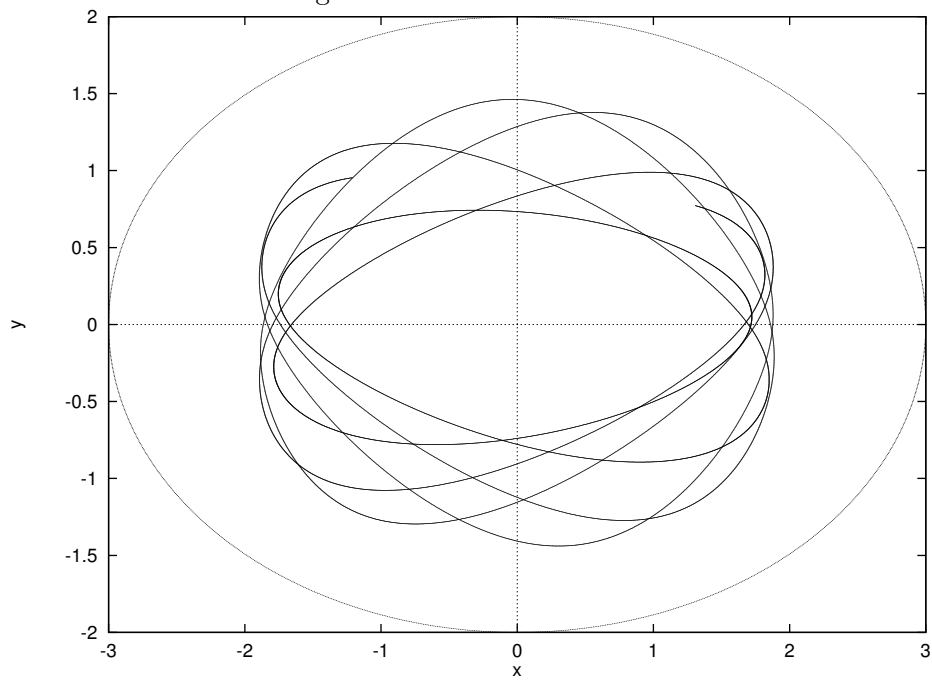
The figures come in pairs that have the same initial values and steepness of V . The odd numbered figures are from case (I), the even numbered figures are from case (II).

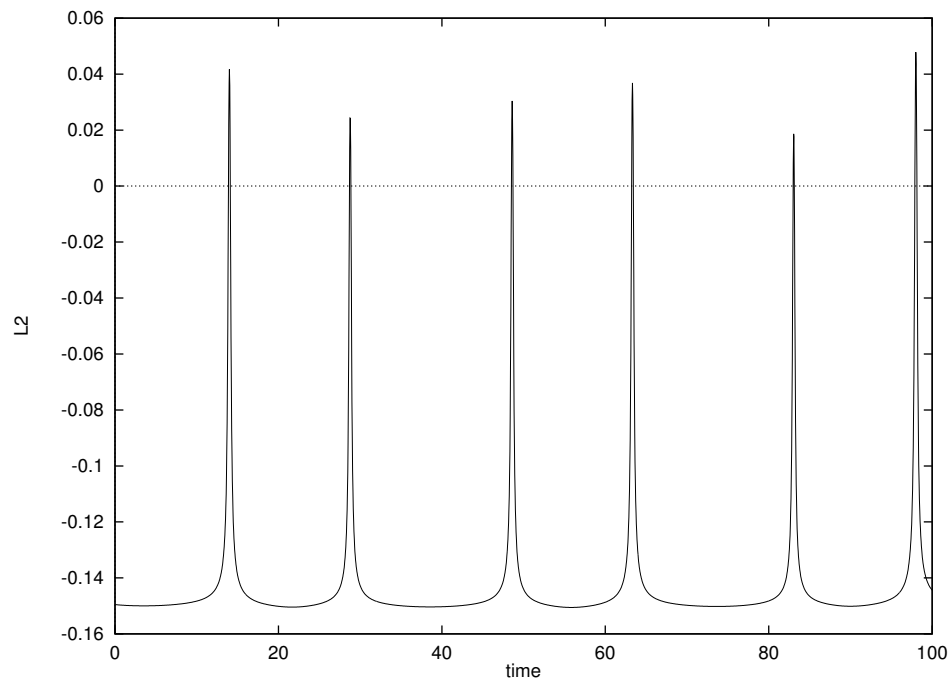
In figures 5 to 8, one sees that – for steep V – the simulation indeed shows the known behavior of the elliptical billiard: the motion is confined to an area either bounded by two hyperbola, lines of constant θ , or bounded by two ellipses, lines of constant z . In figure 9, where \mathcal{L}^2 takes both positive and negative values, but V is the same as in figures 5 to 8, the non-conservation of \mathcal{L}^2 causes a very different behavior from the separable variant in figure 10. This case corresponds to the initial values I discussed in section 1.1.3, namely those for which the initial momentum is nearly parallel to the ellipse. Figures 11 and 12 show what can happen if one makes the potential even less steep. I get strange behavior in case (I), while case (II) is still behaving as I would expect for a billiard system. Of these figures, the last four illustrate most the difference between a z -dependent potential and a potential in which \mathcal{L}^2 is conserved. When \mathcal{L}^2 is conserved, the motion is always restricted to an area bounded by ellipses and hyperbola. In the other case, this need not be so. The simulations confirm the results found in the previous sections. One thing is found from the computer experiments: \mathcal{L}^2 shows a 'dip' or 'peek' when coming close to the boundary, as figure 13 shows. Figure 13 corresponds to the same case as in figure 8, and is a graph of $\mathcal{L}^2(t)$. I see that \mathcal{L}^2 does not approach conserved behavior, but the time-interval where it is not conserved diminishes as $\eta \rightarrow 0$.

Figure 5: Non-conserved \mathcal{L}^2 Figure 6: conserved \mathcal{L}^2

Figure 7: Non-conserved \mathcal{L}^2 Figure 8: conserved \mathcal{L}^2

Figure 9: Non-conserved \mathcal{L}^2 Figure 10: conserved \mathcal{L}^2

Figure 11: Non-conserved \mathcal{L}^2 Figure 12: conserved \mathcal{L}^2

Figure 13: Peeks in \mathcal{L}^2

1.3 Summary

In this part of the thesis, I investigated whether the elliptical billiard has a second constant of motion. The quantity \mathcal{L}^2 which is seen to be conserved, proved to have an ill-defined value of the Poisson-brackets with the Hamiltonian \mathcal{H} , not necessarily zero. By adding a term $X(\vec{x})$, to this quantity, I get the quantity Z that does have a zero value of its Poisson-brackets with \mathcal{H} . X depends on the potential that has to have a certain form to allow for such a quantity. In the construction, V was required to be continuously differentiable, but there exists a limit in which V approaches the hard wall potential. In that case $X = V$, so $Z = \mathcal{L}^2$ inside the ellipse, which explains why a could get \mathcal{L}^2 as a conserved quantity on geometrical grounds. So I conclude that the elliptical billiard is (classically) integrable. Apart from the billiard, I constructed a class of integrable Hamiltonian systems that also have a conserved quantity Z . If V is not of the form required to be in this class, there seems to be no second constant of motion, as the numerical experiments show. The numerical experiments also correctly show that when the potential is of the required form, the motion is confined within the expected bounds, which have the form of hyperbola and ellipses.

2 Quantum-Mechanical Part

In this part I will treat the quantum-mechanical elliptical billiard. In the first section, I explain some theory regarding "quantum chaos", also called "Quantum Chaology", since in a strict sense chaos does not exist in quantum mechanics. In the second section, the elliptical billiard will be discussed and I'll try to get some analytical results. The eigenvalues of the Hamiltonian will turn out to be inaccessible analytically, therefore two sections follow that approach the problem via approximations for asymptotically high energies, and for low-energies, respectively, which give some numerical results. At the end of this part I will give an overall picture of the quantum-mechanical elliptical billiard in the summary.

2.1 Quantum Chaology

2.1.1 Characteristics of Chaotic and Regular Spectra

There are some characteristics of spectra which indicate whether the system is (classically) *regular* or *chaotic*. The main and most tangible characteristics have to do with level spacings: the difference in energy between two subsequent levels.

The first of those characteristics is that of *level crossing versus level repulsion*. On varying a parameter of the system, the energy levels will change. Two levels may get close to each other. In regular systems the levels will then generically come to cross, that is, they become degenerate, while in chaotic systems they should avoid crossing, and show a repulsive behavior. Why this is plausible, I will explain after mentioning the second characteristic, which is the *distribution of level spacings*, defined such that $P(s)ds$ is the probability of having an energy spacing between s and $s + ds$. This distribution is very different for regular and chaotic spectra, not surprisingly, since the first characteristic implies the $P(0) = 0$ for chaotic spectra, while $P(0)$ is finite positive for regular spectra.

Apart from $P(s)$, there is another statistical quantity that can give some indication whether the system is integrable or not, namely the *spectral rigidity* $\bar{\Delta}_3(L)$. This is defined as the deviation of the best fit of $N(E)$ – which is the number of energy-levels with energy smaller than E – over an interval of L mean level spacings to a straight line, averaged over the spectrum,

$$\bar{\Delta}_3(L) = \left\langle \frac{1}{L} \int_{E-L/2}^{E+L/2} (N(E') - a - bE')^2 dE' \right\rangle$$

in which $a + bE'$ should be the best fit of $N(E')$ in $[E - L/2, E + L/2]$ in a least-square sense, so actually

$$\bar{\Delta}_3(L) = \left\langle \min_{(a,b)} \frac{1}{L} \int_{E-L/2}^{E+L/2} (N(E') - a - bE')^2 dE' \right\rangle \quad (2.1)$$

In appendix B.5 the following properties of $\bar{\Delta}_3$ are derived:

$$\bar{\Delta}_3(L_1 + L_2) \geq \frac{L_1}{L_1 + L_2} \bar{\Delta}_3(L_1) + \frac{L_2}{L_1 + L_2} \bar{\Delta}_3(L_2) \quad (2.2)$$

$$\frac{d}{dL} (L\bar{\Delta}_3(L)) \geq 0 \quad (2.3)$$

$$\bar{\Delta}_3(nL) \geq \bar{\Delta}_3(L) \quad n \text{ positive integer} \quad (2.4)$$

One usually applies a transformation to the spectrum such that the average level spacing is one, called unfolding. This is discussed in the next section. For some specific cases, $\bar{\Delta}_3$ can be calculated:

$$\begin{aligned} L < 1: \quad \bar{\Delta}_3(L) &= \frac{L}{15} \\ \text{random spectrum:} \quad \bar{\Delta}_3(L) &= \frac{L}{15} \\ \text{harmonic oscillator:} \quad \bar{\Delta}_3(L) &= \frac{1}{12} - \frac{1}{60L^2}, \quad L \text{ integer} \end{aligned}$$

A regular spectrum is supposed to have uncorrelated levels, and should therefore obey the result for a random spectrum. However, as the result for the harmonic oscillator shows, at some point the structure in the spectrum makes $\bar{\Delta}_3$ saturate. That this is always the case for spectra determined by n numbers is argued in appendix B.5. For chaotic spectra, however, no saturation should take place.

These characteristics can be justified by making an approximation of the total Hamiltonian to a two-by-two submatrix when two levels come close together. That such an approximation is possible is shown in appendix B.2.

For chaotic systems, the characteristics are justified by the conjecture that the behavior of the levels of a chaotic system can be described by ensemble-averages over an ensemble of matrices, so-called *random matrices* (Mehta[17], Haake[13]). The matrices and the measure on them are restricted so as to mirror the symmetries of the system, e.g. the matrices should be Hermitian. Now I can look at the behavior of a two dimensional Hamiltonian

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{12}^* & H_{22} \end{pmatrix} \quad (2.5)$$

The eigenvalues are easily calculated to be

$$E = \frac{H_{11} + H_{22}}{2} \pm \frac{1}{2}\Delta E$$

where

$$\Delta E = \sqrt{(H_{11} - H_{22})^2 + 4 |H_{12}|^2} \quad (2.6)$$

For degenerate levels this will have to be zero, so

$$\begin{aligned} H_{11} - H_{22} &= 0 \\ \text{Re}(H_{12})^2 &= 0 \\ \text{Im}(H_{12})^2 &= 0 \end{aligned} \quad (2.7)$$

An arbitrary Hamiltonian has four independent parameters (H_{11} , H_{22} , H_{12} , H_{12}^*), and there are three requirements to be fulfilled. When a single external

parameter is changed, the independent parameters will in general not satisfy those simultaneously: ΔE has a minimum, rather than a zero. This is what is meant by repelling levels. In the context of *random matrix theory*, an ensemble of Hamiltonians is taken, of which matrices which satisfy (2.7) are but a small subset, of measure zero, so level repulsion will be seen there too.

For a system which has an extra conserved quantity \mathcal{L}^2 , this can change. One can always choose a basis upon which \mathcal{L}^2 is diagonal. If the two approaching levels belong to different values of \mathcal{L}^2 , H will be diagonal too:

$$H = \begin{pmatrix} H_{11} & 0 \\ 0 & H_{22} \end{pmatrix} \quad (2.8)$$

To have $\Delta E = 0$, I now only need

$$H_{11} - H_{22} = 0$$

This can generally be accomplished by varying only one external parameter. Thus, on varying that parameter, one will see crossing of the levels. If the two levels correspond to the same value for \mathcal{L}^2 , then \mathcal{L}^2 is always diagonal (in the two by two approximation), and there is no need for H to be diagonal. The general form is then (2.5) again, and I find again level repulsion. In two dimensions, this avoiding of levels with the same value of \mathcal{L}^2 is to be expected, since if the levels would cross, one would have two states with the same quantum numbers: the values E and λ would not designate the states uniquely, as they should.

For chaotic systems, I can use random matrix theory to find $P(s)$ [13, 17]. First, I need to establish the probability density $P(H)$ for the ensemble of Hamiltonians. I will only consider the *Gaussian ensemble* of hermitian matrices¹ which are of the form (2.5). Besides having to be normalized to unity, there are two other requirements:

- The density should be insensitive to a change of base, so $P(H) = P(U^\dagger H U)$ where U is a unitary matrix;
- The distribution should be such that H_{11} , H_{22} and H_{12} are independent, so

$$P(H) = P_{11}(H_{11})P_{22}(H_{22})P_{12}(H_{12}, H_{12}^*) \quad (2.9)$$

In appendix B.3 it is shown that this restricts the form of $P(H)$ to

$$P(H) = C \exp\left(-A \operatorname{Tr} H^2\right) \quad (2.10)$$

This distribution is in terms of H_{11}, H_{22}, H_{12} and H_{12}^* . The corresponding distribution of eigenvalues is (appendix B.3)

$$P(E_+, E_-) = C(E_+ - E_-)^2 e^{-A(E_+^2 + E_-^2)} \quad (2.11)$$

¹Gaussian Unitary Ensemble, also called GUE.

From this, the level spacing distribution can easily be obtained, which is done in appendix B.4. The result is

$$P(s) = \begin{cases} \frac{32}{\pi^2} s^2 e^{-\frac{4}{\pi}s^2} & \text{unitary, GUE} \\ \frac{\pi}{2} s e^{-\frac{\pi}{4}s^2} & \text{orthogonal, GOE} \\ \frac{2^{18}}{3^6\pi^3} s^4 e^{-\frac{64}{9\pi}s^2} & \text{symplectic, GSE} \end{cases} \quad (2.12)$$

From $P(0) = 0$, one sees that these spectra show level repulsion. For regular spectra, a slightly different approach is necessary, which is also discussed in the appendix, where I get

$$P(s) = e^{-s} \quad (2.13)$$

based on the independence of the energy levels. Therefore this distribution for level spacings is the expected distribution for regular spectra, which is often called the *Poisson distribution* in this context.

Random Matrix Theory also predicts the form of $\bar{\Delta}_3(L)$, to be

$$\begin{aligned} \bar{\Delta}_3(L) &= \frac{1}{\pi^2} \left[\ln(2\pi L) + \gamma - \frac{\pi^2}{8} - \frac{5}{4} \right] & \text{for GOE} \\ \bar{\Delta}_3(L) &= \frac{1}{2\pi^2} \left[\ln(2\pi L) + \gamma - \frac{5}{4} \right] & \text{for GUE} \end{aligned}$$

where γ is Euler's constant. Notice that no saturation takes place.

From the approximation by a two by two matrix another important feature can be illustrated which is not a physical one, but a numerical one, namely, that level repulsion may seem to be occurring, when levels actually intersect, purely due to computational errors. These errors can accumulate in certain diagonalization methods and are usually not very important, except when one wants to distinguish crossing from repulsion. Look at a general 2 by 2 hamiltonian which is degenerate for $\epsilon = 0$:

$$H = \begin{pmatrix} \lambda - \epsilon h_{11} & \epsilon h_{12} \\ \epsilon h_{12}^* & \lambda + \epsilon h_{22} \end{pmatrix} \quad (2.14)$$

Suppose that h_{11} , h_{12} and h_{22} are all non-zero for $\epsilon = 0$, then I can take their values at $\epsilon = 0$ as an approximation for small ϵ . The level spacing as a function of ϵ is then

$$\Delta E = \epsilon \sqrt{(h_{22} + h_{11})^2 + 4 |h_{12}|^2} \quad (2.15)$$

In which the crossing at $\epsilon = 0$ is obvious. Now suppose one can model the computational errors by adding a term to the matrix H :

$$H' = H + \delta \begin{pmatrix} f & 0 \\ 0 & g \end{pmatrix} \quad (2.16)$$

where δ is the order of the error and f and g are independent and non-zero at $\epsilon = 0$. Then ΔE changes to

$$\Delta E^2 = 4[\epsilon^2 |h_{12}|^2 + \left(\frac{g-f}{2}\delta + \frac{h_{22}+h_{11}}{2}\epsilon\right)^2] \quad (2.17)$$

which has its minimum at

$$\epsilon_0 = -\frac{(g-f)\delta}{2|h_{12}|^2 + (h_{11}+h_{22})^2} \quad (2.18)$$

At this point ΔE^2 is

$$\Delta E_0^2 = [(g-f)\delta]^2 y(h_{11}, h_{12}, h_{22}) \quad (2.19)$$

where y is a function that cannot be zero if h_{12} , h_{11} and h_{22} are non-zero. Thus the levels seem to approach each other no closer than a distance of the order of the computational error δ , provided that $g \neq f$, which will be so if f and g are independent.

2.1.2 Weyl's Law and Unfolding of Spectra

In section 2.1.1, all calculations assumed that the average density of states was unity. For the spectrum $\{E_i\}$ of a given system, this will generally not be the case. To be able to compare such a spectrum with the predictions, I need some procedure to scale the average density to unity. This is called *unfolding*. Simply scaling the whole spectrum by a factor is not a good unfolding procedure, since for many spectra the level density depends on the energy, so the unfolding would depend on the number of levels included in the statistical considerations. A better way of unfolding is using a smooth estimate of the number of states \bar{N} below a certain energy value E , and calling

$$E'_i = \bar{N}(E_i) \quad (2.20)$$

the unfolded spectrum $\{E'_i\}$. Then automatically the average density of states is unity, and so is the average level spacing. I need some way to determine this smoothed number of levels below a fixed energy E . There's a law which gives just that, called *Weyl's Law*, which states roughly that the number of levels below E is proportional to the available space for the particle, here the area of the ellipse. It is possible to get some correction terms, and the final result in two dimensions is (Baltes and Hilf[3]):

$$\bar{N}(E) = \frac{A}{4\pi} \frac{2mE}{\hbar^2} \pm \frac{L}{4\pi} \sqrt{\frac{2mE}{\hbar^2}} + K \quad (2.21)$$

where A is the area of the billiard, L the perimeter and K a constant due to singularities – like corners – in the edge². One could go beyond this approximation with an asymptotic expansion in inverse powers of E to regain the full $N(E)$, but these terms depend much more on particularities of the system, e.g. its periodic orbits (Berry and Howls[5]). For unfolding, however, these term are of no importance.

²The \pm depends on whether one has Dirichlet or Neumann boundary conditions.

2.2 The Elliptical Billiard – Analytical Results

2.2.1 The Quantum-Mechanical Version

I will show that the quantum version of the elliptical billiard has many analogies, including the difficulties, with its classical counterpart. The main difference is a difficulty I will discuss in section 2.2.4. But first of all, let me give the exact problem.

Consider the Hamiltonian

$$\mathcal{H} = \frac{\vec{p}^2}{2m} + V(\vec{x}) \quad (2.22)$$

where

$$\vec{p} = \frac{\hbar}{i} \frac{\partial}{\partial \vec{x}} \quad (2.23)$$

The problem to be solved is finding the eigenvalues of the Hamiltonian:

$$\mathcal{H}\Psi = E\Psi \quad (2.24)$$

with the boundary-condition³

$$\Psi(z = z_b) = 0 \quad (2.25)$$

To be able to use this boundary-condition, I will again use elliptic coordinates as defined in (1.1). It is possible to calculate the Laplace operator Δ using the following shortcut. The transformation to elliptic coordinates is conformal, that is, it preserves angles, since the transformation can be written as a transformation in the complex plane formed by $x + iy$:

$$x + iy = f \cosh(z + i\theta) \quad (2.26)$$

and any transformation of the complex plane that is analytical, is conformal. For conformal transformations it can be easily shown that

$$\frac{\partial^2 \Phi(x, y)}{\partial z^2} + \frac{\partial^2 \Phi(x, y)}{\partial \theta^2} = \left[\left(\frac{\partial x}{\partial z} \right)^2 + \left(\frac{\partial x}{\partial \theta} \right)^2 \right] \left(\frac{\partial^2 \Phi(x, y)}{\partial x^2} + \frac{\partial^2 \Phi(x, y)}{\partial y^2} \right) \quad (2.27)$$

So from (1.1) I see

$$\Delta_{x,y} = \frac{1}{f^2 M(z, \theta)} \Delta_{z,\theta} \quad (2.28)$$

With this result, I find for the eigenvalue problem for E in elliptic coordinates

$$\frac{-\hbar^2}{2mf^2 M(z, \theta)} \Delta \Psi = (E - V(z, \theta)) \Psi \quad (2.29)$$

Multiplying this equation with $M(z, \theta)$, I end up with a separable equation again if V is of the form (1.26), and

$$\Psi(z, \theta) = N(z)\Theta(\theta) \quad (2.30)$$

³If $V \neq 0$ then Ψ should be normalizable.

I can separate the eigenvalue problem for E , so that (2.29) becomes

$$\frac{-\hbar^2}{2mf^2}[N\Theta_{\theta\theta} + \Theta N_{zz}] = E[-N \cos^2 \theta \Theta + \Theta \cosh^2 z N] - \Theta V_1 N - N V_2 \Theta$$

The subscripts denote differentiation. This gives

$$\begin{aligned} \frac{-\hbar^2}{2mf^2}\Theta_{\theta\theta} &= [-E \cos^2 \theta + \kappa - V_2]\Theta \\ \frac{-\hbar^2}{2mf^2}N_{zz} &= [E \cosh^2 z - \kappa - V_1]N \end{aligned}$$

or, calling $\frac{2\hbar^2 q}{mf^2} = E$ and $\frac{\hbar^2(a+2q)}{2mf^2} = \kappa$,

$$\Theta_{\theta\theta} + (a - 2q \cos 2\theta) \Theta = \frac{2mf^2}{\hbar^2} V_2 \Theta \quad (2.31)$$

$$N_{zz} - (a - 2q \cosh 2z) N = \frac{2mf^2}{\hbar^2} V_1 N \quad (2.32)$$

For $V_1 = V_2 = 0$, these equations are known as *Mathieu's equation* and *Mathieu's modified equation*, respectively. The above form is called the canonical form. Equation (2.25) does not sufficiently show the nature of the boundary conditions, therefore I will now go into the details of the boundary-conditions when solutions of the separable form (2.30) are sought. It is obvious that Θ has to be a periodic function, so periodic boundary-conditions are imposed on Θ . But it is known that if a mirror-transformation M along some line (or plane in three dimensions) commutes with \mathcal{H} , the eigenfunctions are either symmetric or antisymmetric about that line, since there exist simultaneous eigenfunctions of \mathcal{H} and M . Here both the x -axis as the y -axis provide such mirrors. So I can restate the problem in the following manner. I will look only at the wave functions in the first quadrant: $x > 0$, $y > 0$ or $z > 0$, $0 < \theta < \frac{\pi}{2}$. The boundary then consists of

- the positive x -axis: b_x
- the positive y -axis: b_y
- the line $z = z_b$: b_z

In the following I will denote a *Dirichlet* boundary-condition, $\Psi(b) = 0$, by $D[b]$ and a *Neumann* boundary-condition, $\hat{n} \cdot \nabla \Psi = 0$, by $N[b]$. There is always a boundary-condition $D[b_z]$. Furthermore, Ψ is symmetric or anti-symmetric about the x -axis, so $N[b_x]$ or $D[b_x]$ holds, and the same can be said about the y -axis: $N[b_y]$ or $D[b_y]$. This results in four possible boundary-conditions. Since the x -axis consists of both $z = 0$ and $\theta = 0$, the conditions at those points have to agree. The boundary-conditions expressed in elliptic coordinates thus become (see figure 14)

- (+,g) $N[b_x], N[b_y] \rightarrow N[z = 0], N[\theta = 0], N[\theta = \pi/2]; D[z = z_b]$
- (+,u) $N[b_x], D[b_y] \rightarrow N[z = 0], N[\theta = 0], D[\theta = \pi/2]; D[z = z_b]$
- (-,g) $D[b_x], D[b_y] \rightarrow D[z = 0], D[\theta = 0], D[\theta = \pi/2]; D[z = z_b]$
- (-,u) $D[b_x], N[b_y] \rightarrow D[z = 0], D[\theta = 0], N[\theta = \pi/2]; D[z = z_b]$

where I've labeled the different types indicating with + or - the symmetry or antisymmetry about the x -axis and with g or u the symmetry or antisymmetry under $(x, y) \rightarrow (-x, -y)$ (gerade/ungerade). Current theory regarding quan-

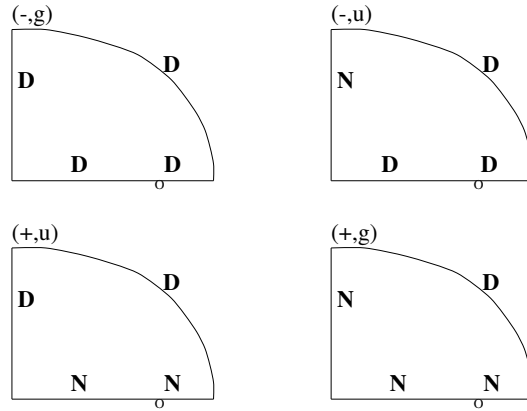


Figure 14: Boundary conditions

tum chaos suggests that classical chaos manifests itself quantum-mechanically in the distribution of the separation of high-lying – semi-classical – energy-levels. So I want a lot of the higher-lying energy levels to be able to do some statistics on the energy level spacings.

2.2.2 The Same Problem

I expect \mathcal{L}^2 to be conserved in the quantum case in the same problematic way as in the classical case, so I calculated the commutator $[\mathcal{H}, \mathcal{L}^2]$. I know that T commutes with all angular momenta, so I have

$$[\mathcal{H}, \mathcal{L}^2] = [V, \mathcal{L}^2] \quad (2.33)$$

I now need \mathcal{L}^2 expressed in elliptic coordinates. Rather than calculating this, I take the classical expressions (1.9) and check them in the quantum mechanical case, interpreting p_z and p_θ as $-i\hbar \frac{\partial}{\partial z}$ and $-i\hbar \frac{\partial}{\partial \theta}$. Note from (1.8) that the following relations also determine l_1 and l_2

$$\begin{aligned} l_1 + l_2 &= 2l_z \\ l_1 - l_2 &= -2fp_y \end{aligned} \quad (2.34)$$

where $l_z = xp_y - yp_x$. The quantities on the right hand sides are easily expressed in elliptic coordinates using the Jacobi matrix

$$\frac{\partial(z, \theta)}{\partial(x, y)} = \frac{1}{M(z, \theta)} \begin{pmatrix} \sinh z \cos \theta & \cosh z \sin \theta \\ -\cosh z \sin \theta & \sinh z \cos \theta \end{pmatrix} \quad (2.35)$$

giving

$$\begin{aligned} 2l_z &= 2 \frac{\cosh z \sinh z p_\theta + \cos \theta \sin \theta p_z}{M(z, \theta)} \\ -2p_y &= -2 \frac{\sin \theta \cosh z p_z + \cos \theta \sinh z p_\theta}{M(z, \theta)} \end{aligned}$$

Calculating $l_1 \pm l_2$ from (1.9) gives me the same expressions, so I conclude that the classical expressions (1.9) are valid in the quantum-mechanical case too. From these, I have to calculate \mathcal{L}^2 . However, just taking $\mathcal{L}^2 = l_1 l_2$ won't do, since it is not hermitian. Therefore I take

$$\mathcal{L}^2 = \frac{1}{2}(l_1 l_2 + l_1 l_2) \quad (2.36)$$

Calculating this is no longer as trivial as it was in the classical case. After the rather lengthy calculation – which I won't do here – I found that \mathcal{L}^2 expressed in elliptic coordinates gives the classical expression (1.10)⁴. Taking V independent on θ again, I now find

$$\begin{aligned} [V, \mathcal{L}^2] &= -\frac{\sin^2 \theta}{M(z, \theta)} [V, p_z^2] + \frac{\sinh^2 z}{M(z, \theta)} [V, p_\theta^2] \\ &= \frac{\hbar^2 \sin^2 \theta}{M(z, \theta)} [V, \frac{\partial^2}{\partial z^2}] - \frac{\hbar^2 \sinh^2 z}{M(z, \theta)} [V, \frac{\partial^2}{\partial \theta^2}] \\ &= -\frac{\hbar \sin^2 \theta}{M(z, \theta)} (\hbar \frac{\partial^2 V}{\partial z^2} + 2 \frac{\partial V}{\partial z} i p_z) \\ &\quad + \frac{\hbar \sinh^2 z}{M(z, \theta)} (\hbar \frac{\partial^2 V}{\partial \theta^2} + 2 \frac{\partial V}{\partial \theta} i p_\theta) \end{aligned} \quad (2.37)$$

The second derivatives are not essential: I could approximate a hard-wall potential using only straight lines, in which case the second derivative would vanish. There remains however, just as in the classical case, a term linear in both p_z as the derivative of V , which becomes infinite at the boundary. So I have here the same problem I had in section 1.1.3. In the classical case this could be solved using a potential of the form (1.26) and adding X to \mathcal{L}^2 . In the next section I will show that this is also possible in the quantum-mechanical case.

2.2.3 Proof that $\mathcal{L}^2 + X$ is a Conserved Quantity

In this section I will prove that $\mathcal{L}^2 + X$ is a *conserved quantity* both classically and quantum-mechanically by calculating the Poisson brackets and the commutator with the Hamiltonian simultaneously. I will use that I already know that \mathcal{L}^2 commutes with T and that X and V commute, since they are both functions of z and θ . Thus

$$[\mathcal{L}^2 + X, T + V] = [\mathcal{L}^2, V] - [T, X] \quad (2.38)$$

⁴This is a surprise only to a certain extend. It turns out that (1.10) is Hermitian when interpreted as an operator, so its factors, which are the same as those of the classical quantity, are in a correct order.

where I mean by $[,]$ both the Poisson-brackets and the commutator. I take V to be of the form (1.26), and X to be (1.27). To make the proof somewhat more transparent, I make the following definitions:

- $P_1 = \frac{p_z^2}{M}, P_2 = \frac{p_\theta^2}{M}$ are momenta squared,
- $F_1 = \sinh^2 z, F_2 = \sin^2 \theta$ are some factors,
- $W_1 = \frac{V_1}{M}, W_2 = \frac{V_2}{M}$ contain the potential,
- $\kappa = [T, X]$

then I have

$$\begin{aligned} [\mathcal{L}^2 + X, T + V] &= [\mathcal{L}^2, V] - \kappa \\ \kappa &= [P_1, F_1 W_2] - [P_1, F_2 W_1] + [P_2, F_1 W_2] - [P_2, F_2 W_1] \end{aligned} \quad (39)$$

Now the following proposition is very useful to bring the F 's over to the other side of the brackets:

Proposition 2.1 *If $[,]$ is the notation for Poisson-brackets or commutators, then*

$$[P, FW] = [PF, W] + W[P, F] + [W, F]P \quad (2.40)$$

Proof: I will prove the proposition for commutators and Poisson-brackets separately:

- *Commutators:*

$$\begin{aligned} [P, FW] - [PF, W] &= PFW - FW P - PF W + W PF = WPF - FWP \\ W[P, F] + [W, F]P &= WPF - WFP + WF P - FW P = WPF - FWP \end{aligned}$$

- *Poisson brackets:*

$$\begin{aligned} [P, FW] - [PF, W] &= [P, F]W + F[P, W] - P[F, W] - [P, W]F \\ &= [P, F]W - P[F, W] \\ &= W[P, F] + [W, F]P \end{aligned}$$

□

Note that because of my definitions I will always have $[F, W] = 0$. With this proposition, using that $[P_1, F_2] = [P_2, F_1] = 0$, I find that

$$\begin{aligned} \kappa &= [P_1 F_1, W_2] - [P_1 F_2, W_1] \\ &+ [P_2 F_1, W_1] - [P_2 F_2, W_1] \\ &+ W_2 [P_1, F_1] - W_1 [F_2, P_2] \end{aligned} \quad (2.41)$$

Since P_2 is a function of θ and V_1 is a function of z , I also know that (since $F_1 + F_2 = M(z, \theta)$)

$$\begin{aligned} 0 &= [P_2, V_1] = [P_2, (F_1 + F_2)W_1] \\ &= [P_2(F_1 + F_2), W_1] + W_1 [P_2, F_2] \end{aligned}$$

and with a similar argument,

$$\begin{aligned} 0 &= [P_1, V_2] = [P_1, (F_1 + F_2)W_2] \\ &= [P_1(F_1 + F_2), W_2] + W_2[P_1, F_1] \end{aligned}$$

So I can add $[P_2, V_1] - [P_1, V_2]$ to κ_2 without altering it. This causes many cancellations leaving me with

$$\kappa = [P_2F_1 - P_1F_2, W_1 + W_2] \quad (2.42)$$

Using $V = W_1 + W_2$ I finally find

$$[\mathcal{L}^2 + X, \mathcal{H}] = [\mathcal{L}^2 - (P_2F_1 - P_1F_2), V]$$

But I already had an expression for \mathcal{L}^2 , and this is exactly $P_2F_1 - P_1F_2$, so the commutator, as well as the Poisson brackets, vanishes:

$$[\mathcal{L}^2 + X, \mathcal{H}] = 0 \quad (2.43)$$

□

2.2.4 Equivalence of the Eigenvalue-problems of \mathcal{L}^2 and E

In many cases the knowledge of an additional conserved quantity A , due to separability, makes it easier to find eigenfunctions of \mathcal{H} . This is because one can then look for eigenfunctions of A , and look for suitable functions that are eigenfunctions of \mathcal{H} and A simultaneously (the circular billiard is a good example of this). However, the knowledge that Z is conserved does not help me any further, as I will show now.

By elementary manipulations (2.31) and (2.32) can be written in the form

$$\hbar^2\Theta_{\theta\theta} + (4q\hbar^2\sin^2\theta + \lambda)\Theta = 2mf^2V_2\Theta \quad (2.44)$$

$$\hbar^2N_{zz} + (4q\hbar^2\sinh^2z - \lambda)N = 2mf^2V_1N \quad (2.45)$$

where $\lambda = (-2q + a)\hbar^2$. The boundary-conditions were developed in section 2.2.1 and mirror a usual *classification* of Mathieu's functions. I now look at the eigenvalue problem of Z , which is

$$\frac{\sinh^2z(p_\theta^2 + 2mf^2V_2) - \sin^2\theta(p_z^2 + 2mf^2V_1)}{M(z, \theta)}\Psi = \lambda\Psi \quad (2.46)$$

After a little rearranging this becomes

$$\frac{\frac{(p_\theta^2 + 2mf^2V_2)}{\sin^2\theta} - \frac{(p_z^2 + 2mf^2V_1)}{\sinh^2z}}{\frac{1}{\sinh^2z} + \frac{1}{\sin^2\theta}}\Psi = \lambda\Psi \quad (2.47)$$

which can be separated:

$$\frac{(p_\theta^2 + 2mf^2V_2)}{\sin^2\theta}\Theta = \left[\frac{\lambda}{\sin^2\theta} + c\right]\Theta \quad (2.48)$$

$$\frac{-(p_z^2 + 2mf^2V_1)}{\sinh^2z}N = \left[\frac{\lambda}{\sinh^2z} - c\right]N \quad (2.49)$$

or

$$\hbar^2 \Theta_{\theta\theta} + [\lambda + c \sin^2 \theta] \Theta = 2mf^2 V_2 \Theta \quad (2.50)$$

$$-\hbar^2 N_{zz} + [\lambda - c \sinh^2 z] N = -2mf^2 V_1 N \quad (2.51)$$

Putting $c = 4\hbar^2 q$, I end up with the same problem as in (2.44) and (2.45), only now the eigenvalue and separation constant have traded places (the boundary-conditions remain unchanged). Therefore, all the difficulties in (2.44) and (2.45), the gravest one being the fact that q and λ appear in both equations, are also present in (2.50) and (2.51), and all I learned was that q , a and λ are real because \mathcal{H} and \mathcal{L}^2 are hermitian. For the problems to be really equivalent, the boundary conditions have to be the same. The boundary conditions of \mathcal{H} can be thought of as arising from a potential V that is a infinite step function. The same has to be done for \mathcal{L}^2 . I have to add X to \mathcal{L}^2 to make it really conserved. This also imposes the boundary conditions for \mathcal{L}^2 , since X is infinite at the boundary and beyond, so the wave functions are forced to be zero on the boundary. As in the classical case, the inclusion of X not only makes \mathcal{L}^2 formally conserved, but also makes the boundary manifest.

2.2.5 Sturm-Liouville Boundary Problems

Finding many energy levels by diagonalizing a finite matrix-approximation, e.g. by discretizing spacial positions, turned out to be not very tractable; I had to turn to the theory of Mathieu-functions to get some results. Since the Mathieu equations are examples of the larger class of *Sturm-Liouville* problems, I will first go into those. The theory I discuss here can be found in Sagan[22].

Let's look at a differential equation

$$Dy = 0 \quad (2.52)$$

with D a differential operator of second order. Let D be self-adjoint, so that it has to be of the form⁵

$$D = \frac{d}{dx} p(x) \frac{d}{dx} + q(x) \quad (2.53)$$

where p is differentiable and p and q are both continuous. Furthermore it is assumed that $p(x) > 0$ for all x in the domain $[a, b]$. It can be shown that zero's of nontrivial solutions of (2.52) are all simple⁶. (2.52) can be made into a boundary problem by imposing boundary conditions at x_1 and x_2 inside $[a, b]$. However, the problem thus constructed has solutions only for certain $q(x)$. So it makes sense to write

$$q(x) = Q(x) + \lambda R(x) \quad (2.54)$$

so $q(x)$ can be varied, and one can look for λ s for which the boundary problem has a solution. It will be assumed that $R(x) > 0$ for all x (inside $[a, b]$). This

⁵To be interpreted in an operator-sense: $\frac{d}{dx}$ operates on everything to its right.

⁶i.e. $y(x) = 0$ implies $y'(x) \neq 0$.

problem is called a Sturm-Liouville problem and the values of λ for which the problem has a solution are called *eigenvalues* (sometimes characteristic values) and the solution itself is called an *eigenfunction*. The Sturm-Liouville problem can also be seen as the eigenvalue problem of the operator

$$\tilde{D} = \sqrt{R(x)}^{-1} \frac{d}{dx} p(x) \frac{d}{dx} \sqrt{R(x)}^{-1} + [R(x)]^{-1} Q(x) \quad (2.55)$$

which is also hermitian, so the eigenvalues are real. The eigenfunctions $v(x)$ of this problem are related to the $y(x)$ via

$$v(x) = \sqrt{R(x)} y(x) \quad (2.56)$$

Note the importance of $R(x)$ being positive. Indeed the Sturm-Liouville problem is known to have an infinite number of eigenvalues $\lambda_1 < \lambda_2 < \lambda_3 < \dots$, which are all simple (non-degenerate). If $y(x, \lambda_k)$ is the solution corresponding with the k th eigenvalue λ_k , then $y(x, \lambda_k)$ has one more zero in $[x_1, x_2]$ than $y(x, \lambda_{k-1})$. Furthermore $\lim_{k \rightarrow \infty} \lambda_k = \infty$. For Dirichlet boundary conditions, the first eigenfunction (the ground state) will have no zero's between x_1 and x_2 .

I will modify the Sturm-Liouville problem slightly by making $Q(x)$ linearly dependent on a second, 'external', *parameter*:

$$Q(x) = \xi K(x) + S(x) \quad (2.57)$$

There is no need for $K(x)$ to be sign definite, in contrast with the coefficient R of λ . The eigenvalues λ_k will now become functions of ξ : $\lambda_k = \lambda_k(\xi)$. Since the eigenvalues λ_k all exist for every ξ , they form a set of lines in the (λ, ξ) -plane, called characteristic curves, which do not intersect, otherwise the corresponding solution would have both k and $k + 1$ zero's, a clear contradiction. The lines can be seen as solutions of the equation

$$y(x_2, \lambda, \xi) = 0 \quad \Rightarrow \quad \lambda = \lambda_k(\xi) \quad (\lambda_k(\xi_0) = \lambda_0 \text{ fixed}) \quad (2.58)$$

where y is a solution of (2.52) with parameters set to λ and ξ , with initial value set by the boundary condition at x_1 , but without a condition at x_2 ⁷. To say anything about continuity of $\lambda_k(\xi)$, I need the implicit function theorem which states:

Theorem 2.1 *Suppose W is an open subset of $R^{n+p} = R^n \times R^p$. Let f be a continuous, k times differentiable function $W \rightarrow R^n$ ($k > 0$). Furthermore take (a, b) in W , $f(a, b) = 0$ and $\frac{\partial f}{\partial x}(a, b): R^n \rightarrow R^n$ invertible ((x, y) in $R^n \times R^p$). Then there exists an open environment A of a in R^n and an open environment B of b in R^p such that for every y in B there is precisely one $x = \Psi(y)$ in A that satisfies $f(x, y) = 0$. Furthermore Ψ is continuous and k times differentiable.*

⁷If $y(x_1) = 0$, because of the simplicity of the zero's, $y'(x_1) \neq 0$, so in that way I can get the two initial conditions needed to make the solution of a second order differential equation unique.

Thus $\lambda_k(\xi)$ is continuous provided that

$$\frac{\partial y}{\partial \lambda} \neq 0 \quad (2.59)$$

Now if $\frac{\partial y}{\partial \lambda} = 0$ this should occur only at an isolated point $\lambda = \lambda^*$, otherwise $y(x_2, \lambda, \xi)$ would be flat in the λ -direction and since $y(x_2, \lambda_0, \xi_0) = 0$, this would mean that all λ s in that region are eigenvalues, which contradicts the earlier statement that the eigenvalues are simple. Thus the characteristic curves are at least piecewise continuous. Discontinuities of these curves are shown not to exist in appendix C.1, when a restriction is imposed on $K(x)$. This is formulated in theorem 2.2(not found in[22]):

Theorem 2.2 *Consider a Sturm-Liouville problem*

$$\left[\frac{\partial}{\partial x} p(x) \frac{\partial}{\partial x} + \lambda R(x) + \xi K(x) + S(x) \right] y(x) = 0 \quad (2.60)$$

with p positive, continuous differentiable, R , K and S continuous, R positive, and with certain boundary conditions imposed. If there exist a constant c such that $cK(x) < R(x)$, then the characteristic curves $\lambda_k(\xi)$ are continuous functions of ξ .

2.2.6 Theory of Periodic Mathieu Functions

I will now show explicitly how the Mathieu equations can be regarded as Sturm-Liouville problems. The parametrized form under the above definitions looks like (2.60). First, I look at (2.31), and I see that by identifying $x \equiv \theta$, $y \equiv \Theta$, $\lambda \equiv a$, $\xi \equiv q$, and

$$\begin{aligned} p(x) &\equiv 1 \\ R(x) &\equiv 1 \\ K(x) &\equiv -2 \cos 2\theta \\ S(x) &\equiv 0 \end{aligned}$$

it is of the form (2.60). Note that $K(x)$ can be negative in this case, so that a has to be identified as the eigenvalue, not q . The boundary conditions were already discussed in section 2.2.1. In the modified Mathieu equation (2.32) the following identification can be made: $x \equiv z$, $y \equiv N$, $\lambda \equiv q$, $\xi \equiv a$, and

$$\begin{aligned} p(x) &\equiv 1 \\ R(x) &\equiv 2 \cosh 2z \\ K(x) &\equiv -1 \\ S(x) &\equiv 0 \end{aligned}$$

Notice that the parameter and the eigenvalue are interchanged with respect to (2.31).

Mathieu functions, solutions of equation (2.31), are reasonably well documented, e.g. in McLachlan[16] and Arscott[2]. This rest of the section will be a

summary of theorems regarding Mathieu functions. I will not give any proofs, those can be found in Arscott[2, Chapter II]. The numbers the theorems have in Arscott are given in parentheses: the theorems are taken almost literally from it, except for notational differences.

Theorem 2.3 (2 + corollary) *Mathieu's equation always has one even and one odd solution, about any point $z = n\pi/2$ (n integral).*

These correspond to the conditions $D[\theta = 0]$ and $N[\theta = 0]$ and, for $n = 1$, $D[\theta = \pi/2]$ and $N[\theta = \pi/2]$.

Theorem 2.4 (4) *Mathieu's equation always has at least one solution $y(z)$ such that $\Theta(\theta + \pi) = \sigma\Theta(\theta)$, where σ is a constant which depends on the parameters of the equation and which may be real or complex.*

Now I turn specifically to π or 2π periodic solutions of Mathieu's equations, for which the boundary conditions will then be satisfied. These exist if $\sigma = \pm 1$. σ depends on the parameters. I will keep q fixed and let a vary. The values of a for which $\sigma = \pm 1$ are the *characteristic values* or *eigen-values*. At those values periodic solutions can exist. Since I have a second order differential equation, there could be two of those. For $q = 0$ there are two, namely $\sin \sqrt{a}\theta$ and $\cos \sqrt{a}\theta$. The following theorem tells me what happens for other values of q .

Theorem 2.5 (6, 'Ince') *Except in the trivial case $q = 0$, Mathieu's equation never possesses two periodic solutions, such that $\Theta(\theta + \pi) = \pm\Theta(\theta)$, for the same values of q and a .*

From now on, I will mean by periodic solutions, solutions with $\Theta(\theta + \pi) = \pm\Theta(\theta)$. The last result has physical significance. I saw that q represents energy and $a - 2q$ is an eigenvalue of \mathcal{L}^2 . Given some q , suppose I could find a value of a such that there were two periodic solutions of (2.31). For the modified Mathieu equation (2.32), it doesn't matter which one I take. If the solution of the modified Mathieu equation has a zero at some point z_0 , then I get a solution of a problem with the elliptical boundary at $z_b = z_0$, by combining the solution of the modified equation with either one of the solutions of the Mathieu equation. So I would get two independent eigenfunctions of \mathcal{H} , with the same numbers q and a , corresponding to the two independent conserved quantities of the system. These two numbers should, however, suffice to label all quantum levels. Thus physically, this situation is not allowed. The theorem assures me that this situation does not occur. Still, at $q = 0$ the reasoning above breaks down, since then the solutions of the modified Mathieu equation are $\sinh \sqrt{a}\theta$ and $\cosh \sqrt{a}\theta$, which do not have any zero's (except at 0). This also tells me that the ground-state energy, not surprisingly, cannot be equal to zero. It can be shown that as a consequence of this theorem, the periodic Mathieu functions fall into four classes[2]:

- I. Even, period π
- II. Even, period 2π
- III. Odd, period 2π
- IV. Odd, period π

corresponding exactly to the four types $(+, g)$, $(+, u)$, $(-, g)$ and $(-, u)$ respectively, as found in section 2.2.1. Once I have found a relation between a and q (there are several methods to compute them for a given q), the only remaining condition will be $D[b_z]$ on the modified Mathieu equation. How this last condition is solved is discussed in the next few sections. Before a can do that, I need a few properties of the relation between q and a :

Theorem 2.6 (9 + corollary) *When q is real, the values of a which give rise to periodic solutions of Mathieu's equation are all real and different; they are continuous functions of q , finite when q is finite, and reducing for $q = 0$ to $a = n^2$ (n integral). Moreover, the periodic solutions are continuous functions of q for real q , that reduce, for $q = 0$, to multiples of the trigonometric functions $\cos n\theta$, $\sin n\theta$.*

Notice that this is just an application of the theorem in the previous section, about the continuity of the characteristic curves. The curves, starting at $(0, n^2)$, never intersect each other – that would mean that two independent periodic solutions exist. These curves are denoted by a_{2n} for type I solutions, a_{2n+1} for type II, b_{2n+1} for type III and b_{2n+2} for type IV. The corresponding solutions are called ce_{2n} , ce_{2n+1} , se_{2n+1} and se_{2n+2} respectively – inspired by their sine or cosine character near $q = 0$. Actually this character is preserved along a characteristic curve, as formulated in the following theorem:

Theorem 2.7 (10 + corollary) *A periodic solution of Mathieu's equation has the same number of zero's in $0 < \theta < \pi/2$ for all real values of q . This number is n if the solution reduces to $\cos 2n\theta$, $\cos(2n+1)\theta$, $\sin(2n+1)\theta$, $\sin(2n+2)\theta$ for $q = 0$.*

This of course also follows from the theory of the previous section: the curve $a_k(q)$ corresponds to solutions with k zero's.

2.2.7 Complex Reformulation of the Problem

In this section I will develop a picture of the problem at hand formulated in the complex plane. Consider the Mathieu-equation (2.31). Given a value of q , it is known that periodic solutions only exist for a countable set of characteristic values, $a_r(q)$. However, in the problem at hand, q and a are also related through the modified Mathieu equation (2.32) and its boundary conditions. Consider therefore the Mathieu-equations (2.31) and (2.32) and notice that (2.32) can be obtained from (2.31) by substituting iz for θ . I now claim that the combined problem can be replaced by the following problem in the complex plane (Arscott[2, 3.5]):

$$\frac{d^2 \mathcal{M}_{aq}}{dz^2}(z) + (a - 2q \cos 2z) \mathcal{M}_{aq}(z) = 0 \quad (2.61)$$

with "boundary" conditions

$$\mathcal{M}_{aq}(0) = 0 \quad \text{or} \quad \frac{d\mathcal{M}_{aq}}{dz}(0) = 0$$

$$\begin{aligned} \mathcal{M}_{aq}(\pi/2) = 0 \quad \text{or} \quad \frac{d\mathcal{M}_{aq}}{dz}(\pi/2) = 0 \\ \mathcal{M}_{aq}(iz_b) = 0 \end{aligned} \quad (2.62)$$

To prove this, it is enough to see that

- if I substitute $\theta + iz$ for z in (2.61), it reduces to (2.31) on the real axis and to (2.32) on the complex axis;
- the boundary conditions of (2.31) and (2.32) are the same at 0, and the first condition in (2.62) automatically gives these equal conditions on the real and imaginary axis at 0;
- the other conditions in (2.62) are the boundary conditions at $z = z_b$ and $\theta = \pi/2$.

This also means that if I have a solution of (2.31), I can get a solution of (2.61) by analytic continuation. However, it is not guaranteed that the boundary condition at z_b is satisfied. This condition determines which q values are allowed. These allowed q values make up the spectrum of \mathcal{H} , up to a proportionality constant. The eigenfunction is then

$$\langle z, \theta | E = 2\hbar^2/(mf^2)q ; \lambda = \hbar^2(a - 2q) \rangle = \mathcal{M}_{aq}(iz)\mathcal{M}_{aq}(\theta) \quad (2.63)$$

The solutions of the modified Mathieu equation are thus $ce_m(iz)$ and $se_m(iz)$, also called $Ce_m(z)$ and $Se_m(z)$. The equivalence of \mathcal{L}^2 and \mathcal{H} makes it easy to prove the bounds (1.32) on \mathcal{L}^2 are valid in the quantum-mechanical case too. (1.30) and (1.31) still hold. Now I look at

$$\langle E, \lambda | \mathcal{L}^2 + X | E, \lambda \rangle$$

and use (1.30) and (1.31). Using the fact that $|E, \lambda\rangle$ is an eigenfunction of both \mathcal{H} and \mathcal{L}^2 , the bounds can then be found again in a straightforward manner,

$$-2mf^2E \leq \lambda \leq 2mb^2E$$

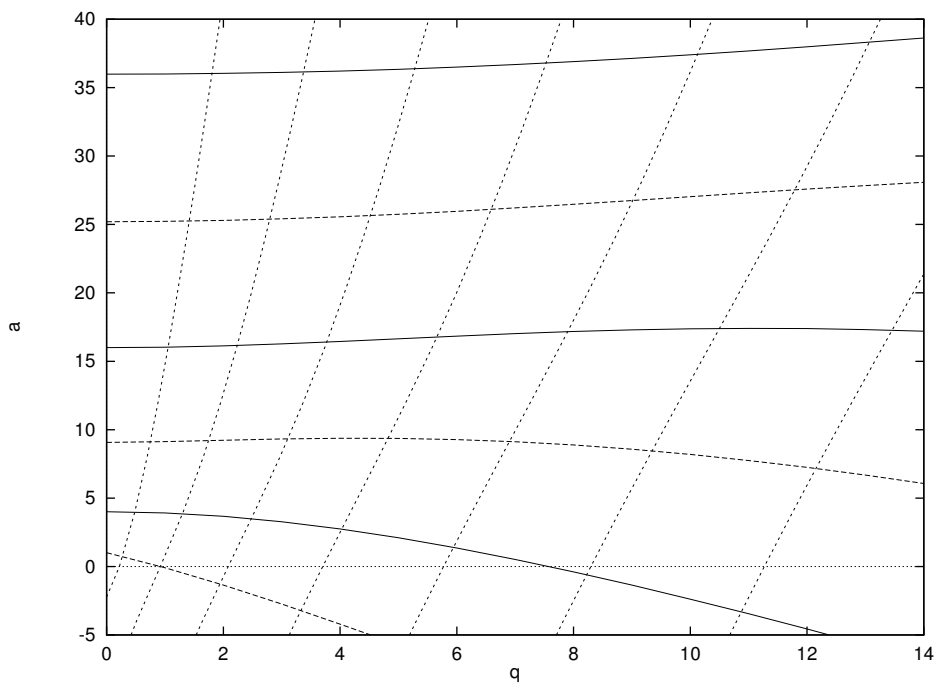
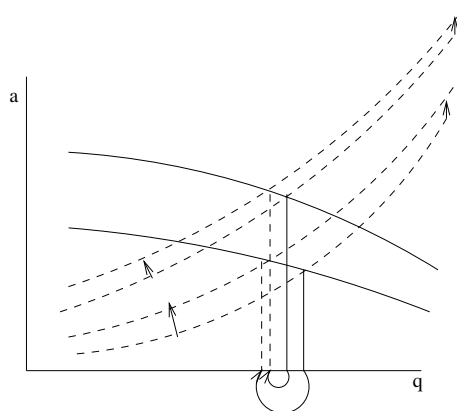
or

$$-2q \leq a \leq 2q\left(2\frac{a^2}{f^2} - 1\right) \quad (2.64)$$

2.2.8 Formulation of the Problem in the (q, a) -Plane

Now I will formulate the problem of the elliptic billiard in terms of objects in the (q, a) plane, which proved to be a very fruitful approach in understanding some of the features that I will find in the approximations in the next sections.

Notice that the characteristic curves in the standard Mathieu equation are functions $a_i(q)$, while those of the modified Mathieu equation are functions $q_j(a)$. A solution of the whole problem (the eigenvalue problem of \mathcal{H} or \mathcal{L}^2) exists for every *intersection point* of those curves in the (q, a) -plane, where $a_i(q_j(a)) = a$ and $q_j(a_i(q)) = q$. Thus every eigenfunction is represented by

Figure 15: Eigenstates in the (q, a) -plane.Figure 16: Dynamics of Eigenstates in the (q, a) -plane.

such an intersection point. The spectrum of \mathcal{H} is now the projection of these points onto the q -axis. This is depicted in figure 15. The vertically oriented curves are the $q_j(a)$, the horizontally oriented curves are the $a_i(q)$. In figure 16, I also showed what happens when the eccentricity is changed. Only the $q_j(a)$ are changed, continuously, and so will the intersection points. Two points at some distance apart will move independently. But they can get close together in the projection on the q -axis. So if these two points approach each other in the projection, there is no reason why they should not proceed in that direction upon further changing of the eccentricity, since in the (q, a) -plane, they do not approach each other at all. Therefore, generically levels will cross on varying the parameter ϵ .

One also sees that the states are labeled according to two *quantum numbers*, namely the numbers of the characteristic curves that intersect. These in turn correspond to the number of zeros of the wave function in the z and the θ -direction.

The lines in figure 15 were found from numerical calculation of the eigenvalues of a Sturm-Liouville problem, as discussed in appendix D.3.

2.3 High Energies – Asymptotic Method

2.3.1 Horn-Jeffreys Asymptotic Method on Mathieu Functions

In the section 2.2.7, I reformulated the problem of finding energy levels and their wave-functions by the problem of finding those pairs $(q, a_r(q))$ such $\mathcal{M}_{aq}(iz_b) = 0$. This problem has no solution that can be written in terms of elementary functions, but it is possible to obtain *asymptotic* results for $q \rightarrow \infty$. The first step will be to construct asymptotic expansions for periodic \mathcal{M}_{aq} . That means that a is – asymptotically – a characteristic value. Not surprisingly, in the method followed here, I will construct asymptotic expansions for $a_r(q)$ and \mathcal{M} simultaneously. The method can be found in McLachlan[16] and Arscott[2]. Therefore I will adopt the standard form that McLachlan uses for the Mathieu-equation

$$y'' + (a - 2q \cos 2z)y = 0 \quad (2.65)$$

The equation is easily rewritten to

$$y'' - (4q \cos^2 z)y + (a + 2q)y = 0 \quad (2.66)$$

From (2.64) I see that a as a function of q can vary at most linearly with q , otherwise the inequality is violated for some q . The right hand side was induced by the boundary-conditions, which shouldn't play any role in finding the characteristic values a because these come from the demand of periodicity. Though the left hand side suggests that in the asymptotic limit $a(q) = -2q$, this cannot really be derived from it. Strictly, I would have to take the general form $a(q) = -\kappa q$ for now, but the derivation is simplified much by assuming that $\kappa = 2$. Later I will show that this value is necessary for consistency.

Now that I have the leading term of $a(q)$, I write

$$a(q) = -2q + \sqrt{q}\beta(q) \quad (2.67)$$

Inserting this into Mathieu's equation gives me

$$y'' - q\left\{4 \cos^2 z - \frac{\beta}{\sqrt{q}}\right\}y = 0 \quad (2.68)$$

I will now argue that $\beta = \mathcal{O}(1)$, so that I am justified to write $a(q)$ in an asymptotic expansion in $k = \sqrt{q}$ as

$$a = -2k^2 + \alpha k + \alpha_0 + \sum_{i=1}^{\infty} \alpha_i k^{-i} \quad (2.69)$$

To find the order of β , I will look at the zero's of solutions of equation (2.68). These lie in the regions where y oscillates, so where

$$4 \cos^2 z - \frac{\beta}{k} < 0$$

Now I investigate the possibility that $\beta = \mathcal{O}(k)$ or worse. Then for large k , y will oscillate everywhere for reasonable β – I need to be able to get some range

of β 's since an infinite sequence of periodic solutions and corresponding a 's, exists for every q , and y will satisfy the approximate equation

$$y'' = -k\beta y$$

having solutions (A and ϕ_0 are constants):

$$y(z) = A \sin(\sqrt{k\beta}z + \phi_0)$$

These solutions have $2\sqrt{k\beta} = \mathcal{O}(k)$ zero's. For k large, the number of zero's thus would get very large. But I already saw in section 2.2.6 that for all q , there exist solutions of the Mathieu equation with r zero's, where r runs from 1 to infinity. So to be able to find those solutions using an asymptotic method, I have to take $\beta = o(k)$. This is consistent with the assumption that the coefficient of the quadratic term in k in the expression for a is -2 , since β cannot contribute to that term anymore. Working with expansions in integer powers of k only, then $\beta = o(k)$ of course implies that $\beta = \mathcal{O}(1)$, as I wanted to show.

Unfortunately, in the method I will use, the coefficient α in (2.69) cannot be determined. There are ways to determine α , but they are beyond the scope of the method. In appendix C.4, I will give one derivation of the result

$$\alpha = 2(2m + 1) \tag{2.70}$$

Here m is an integer constant such that a is an approximation for the characteristic curve corresponding to the solutions ce_m and se_{m+1} which are each other asymptotics. So all solutions, with an arbitrary number of zero's, are a priori equally accessible via an asymptotic method. Often I will use the following two constants

$$\begin{aligned} m_1 &= 2m + 1 \\ m_2 &= m^2 + m + 1 \end{aligned}$$

so then $\alpha = 2m_1$.

The asymptotic method now consists of substituting (2.69) into the equation and equating powers of k . Obviously this doesn't make sense unless I have an asymptotic form of y , too. Consider again (2.68). In the limit of high k , it states

$$y'' - (4k^2 \cos^2 z)y = 0$$

so

$$\left(\frac{y'}{y}\right)' + \left(\frac{y'}{y}\right)^2 = \frac{y''}{y} = \mathcal{O}(k^2)$$

I therefore expect one of the two terms on the left-hand side to be of that same order. However, if $(y'/y)' = \mathcal{O}(k^2)$, then $(y'/y)^2 = \mathcal{O}(k^4)$, which is wrong, so necessarily

$$\left(\frac{y'}{y}\right) = \mathcal{O}(k)$$

which gives the *asymptotic behavior* of y

$$y(z) \sim \zeta(z) \exp(k \chi(z)) \quad (2.71)$$

where $\zeta(z) = \mathcal{O}(1)$ and $\chi(z) = \mathcal{O}(1)$. Now in my asymptotic expansion of y , I could expand both ζ and χ in powers of k^{-1} , but since k^{-1} is small, I could then replace the exponent by its Taylor expansion and incorporate all correction terms of χ in those of ζ . Therefore the most general form for y is already given by

$$y(z) \sim e^{k\chi(z)} \zeta(z) \left[1 + \sum_{i=1}^{\infty} k^{-i} f_i(z) \right] \quad (2.72)$$

which I can now substitute into (2.66). I equate powers of k and find

$$[\chi']^2 = 4 \cos^2 z \quad (2.73)$$

$$2\chi'\zeta' + (\alpha + \chi'')\zeta = 0 \quad (2.74)$$

$$f_i \zeta'' + 2f_i' \zeta' + (f_i'' + 2\chi' f_{i+1}' + \sum_{j=0}^i \alpha_j f_{i-j}) \zeta = 0 \quad (2.75)$$

where I've defined $f_0(z) = 1$. (2.73) gives

$$\chi(z) = \pm 2 \sin z \quad (2.76)$$

the \pm -sign corresponds to the two independent solutions one expects from a second order differential equation. Had I taken $\kappa \neq 2$ then I would have gotten

$$\chi(z) = \int \sqrt{2 - \kappa - 4 \sin^2 z} dz \quad (2.77)$$

This is not periodic unless $\kappa = \pm 2$. $\kappa = -2$ would mean a complex χ , and in principle this should not be necessary since (2.65) is real. I therefore consider only $\kappa = 2^8$. (2.74) can be solved in a straightforward manner, giving

$$\zeta(z) = \frac{1}{\sqrt{\cos z} \tan(z/2 + \pi/4)^{\pm\alpha/4}} \quad (2.78)$$

The constants of integration in χ and ζ only affect the normalization, which can be chosen in any convenient way. The functions $f_i(z)$ can be obtained recurrently from

$$f_{i+1} = - \int^z \frac{f_i \zeta'' + 2f_i' \zeta' + f_i'' + \sum_{j=0}^i \alpha_j f_{i-j}}{2\chi'} dz' \quad (2.79)$$

However, I do not know the α_i , and a method to determine these is required. I will set up a procedure in which at the i -th stage of the approximation, α_0

⁸the negative value actually corresponds to a shift $z \rightarrow \frac{1}{2}\pi - z$ and some normalization.

to α_{i-1} are known when (2.79) is evaluated, and in which α_i follows from the construction of periodic solutions. The unknown term in (2.79) is then

$$\begin{aligned} \int^z \alpha_i \frac{1}{2\chi'} dz' &= \pm \frac{\alpha_i}{2} \int^z \frac{1}{2 \cos z'} dz' \\ &\equiv \pm \frac{\alpha_i}{4} L_1 \end{aligned} \quad (2.80)$$

Where L_1 is defined in appendix C.5. Let me start by looking at stage $i = 0$. Note that all terms in (2.79) can be written in terms of the L_n and I_n of appendix C.5. I was solving Mathieu's equation, looking for periodic solutions. Now L_1 is not periodic and diverges for $z = \pi/2$. In fact, via (C.22), every L_n contains a non-periodic term proportional to L_1 . As seen from (2.80), α_0 appears only in that term. In order that f_1 be periodic, the coefficient in front of L_1 needs to be zero, and in this way I determine what α_0 has to be. The expression for f_1 will then only contain terms like $\sin z \cos^{-n} z$ and $\cos^{-n} z$, whose integrals are I_n and L_n . So in the following step of the approximation, I find from (C.22) an expression containing a L_1 -term, which should be zero, thus fixing α_1 . Thus the procedure of integrating and putting the *logarithmic term* to zero enables me to determine a_i and f_{i+1} to any desired order. At all stages, I have two independent solutions. From (2.76) I see that if one of those is $y^{(1)}(z)$, then the other is $y^{(2)}(z) = y^{(1)}(-z)$, at least in first order. But in (2.79) all terms have this property for $i = 0$, so f_1 has this property of $f_1^{(1)}(z) = f_1^{(2)}(-z)$. Then for f_2 , again all terms have this property. By induction I now see that $y^{(2)}(z) = y^{(1)}(-z)$ to all orders. Evidently *even* and *odd* solutions around $z = 0$ are then

$$y^{(\pm)}(z) = y^{(1)}(z) \pm y^{(2)}(z) \quad (2.81)$$

To find an approximation to ce_{2n} , say, I would have to take $\alpha = 2(2n + 1)$ and calculate the f 's. Then I would have to impose the symmetries of ce_{2n} , so I would need $y^{(+)}$ around $z = 0$. However, the approximation breaks down at $z = \frac{\pi}{2}$, where (2.78) becomes singular. For $-\frac{\pi}{2} < z < \frac{\pi}{2}$, it can be used again, but now I have to impose that $y(\pi + z) = y(\pi - z)$, which means I have to take $y^{(-)}(z)$ there. When looking for eigenvalues q , I will show that this *sign-problem* doesn't cause any trouble. Before proceeding, I will rewrite (2.79) in a convenient way. Performing partial integrations and using (from (2.74))

$$\begin{aligned} \frac{\zeta'}{\zeta} &= \frac{-\alpha - \chi''}{2\chi'} \\ &= \frac{-\frac{\alpha}{2} + \sin z}{2 \cos z} \\ \frac{\zeta''}{\zeta} &= \left(\frac{\zeta'}{\zeta} \right)' + \left(\frac{\zeta'}{\zeta} \right)^2 \\ &= \frac{3 + \frac{\alpha^2}{4}}{4 \cos^2 z} - \frac{\alpha \sin z}{2 \cos^2 z} - \frac{1}{4} \\ &= \frac{m_2 - m_1 \sin z}{\cos^2 z} - \frac{1}{4} \end{aligned}$$

I get for the + -sign case,

$$\begin{aligned}
 f_{i+1} &= -\frac{f'_i(z)}{4 \cos z} + m_1 \frac{f_i(z)}{4 \cos^2 z} - \sum_{j=0}^i \alpha_j \int^z \frac{f_{i-j}(z')}{4 \cos z'} dz' \\
 &\quad - \int^z \frac{f_i(z')}{4 \cos z'} \left[\frac{m_2 + m_1 \sin z'}{\cos^2 z'} - \frac{1}{4} \right] dz'
 \end{aligned} \tag{2.82}$$

Now that the method has been developed, I can go ahead and compute approximations of y . First I determine the *zeroth order functions* from (2.76) and (2.78), finding

$$y_1^0 = \frac{\exp[2k \sin z]}{\sqrt{\cos z} (\tan(z/2 + \pi/4))^{\alpha/4}} \tag{2.83}$$

$$y_2^0 = \frac{\exp[-2k \sin z] (\tan(z/2 + \pi/4))^{\alpha/4}}{\sqrt{\cos z}} \tag{2.84}$$

Using (2.70), and the formulae

$$\begin{aligned}
 [\tan(z/2 + \pi/4)]^{-\frac{1}{2}} &= \sqrt{2} \frac{\cos(z/2 + \pi/4)}{\sqrt{\cos z}} \\
 [\tan(z/2 + \pi/4)]^{\frac{1}{2}} &= \sqrt{2} \frac{\sin(z/2 + \pi/4)}{\sqrt{\cos z}}
 \end{aligned}$$

I can rewrite these to

$$\begin{aligned}
 y_1^0 &= 2^{m+\frac{1}{2}} \exp[2k \sin z] \frac{(\cos(z/2 + \pi/4))^{2m+1}}{\cos^{m+1} z} \\
 y_2^0 &= 2^{m+\frac{1}{2}} \exp[-2k \sin z] \frac{(\sin(z/2 + \pi/4))^{2m+1}}{\cos^{m+1} z}
 \end{aligned} \tag{2.85}$$

The common normalization factor $2^{m+\frac{1}{2}}$ will be left out in subsequent sections.

2.3.2 Higher Orders

Now I compute higher order f 's. I will only compute f_1 here, since it turned out that that term cannot be neglected, while higher orders can. I now only consider the case of $2 \sin z$, the negative case is easily found substituting $-z$ for z . (2.79) becomes

$$f_1 = - \int \frac{\frac{\zeta''}{\zeta} + \alpha_0}{4 \cos z} dz \tag{2.86}$$

After the integration I get

$$f_1 = \frac{1}{32} \left[\frac{-(m_1^2 + 3) \sin z + 4m_1}{\cos^2 z} - (m_1^2 + 1 + 8\alpha_0)L_1 \right]$$

The logarithmic term (L_1) has to be zero, so⁹

$$\begin{aligned}\alpha_0 &= -\frac{m_1^2 + 1}{8} \\ &= \frac{1}{4} - \frac{m_2}{2}\end{aligned}\tag{2.87}$$

and

$$\begin{aligned}f_1(z) &= \frac{4m_1 - (m_1^2 + 3) \sin z}{32 \cos^2 z} \\ &= \frac{m_1 - m_2 \sin z}{8 \cos^2 z}\end{aligned}\tag{2.88}$$

With α_0 given, the recurrence relation for the f_i can be written as

$$\begin{aligned}f_{i+1} &= \frac{m_1}{4 \cos^2 z} f_i(z) - \frac{1}{4 \cos z} f_i'(z) - \frac{\alpha_i}{4} L_1(z) \\ &\quad - \int^z \frac{1}{4 \cos z'} \left\{ f_i(z') \left(\frac{m_2 + m_1 \sin z'}{\cos^2 z'} - \frac{m_2}{2} \right) + \sum_{j=1}^{i-1} \alpha_j f_{i-j}(z') \right\} dz'\end{aligned}\tag{2.89}$$

for $i > 0$.

2.3.3 High-lying Energy Levels

As noted in section 2.2.7 I need those q values for which $\mathcal{M}(iz_b) = 0$. With the result of section 2.7, I can get $\mathcal{M}(iz)$ by substituting iz for z . The denominator $\sqrt{\cos z}$ then becomes $\sqrt{\cosh z}$, so I'm no longer plagued by singularities or the subsequent changes in sign for Ce_{2n} , say¹⁰. The *wave-function* in the angular direction was given by (2.83) in zeroth order. Higher orders give

$$\begin{aligned}y_1(z) &\sim y_1^0 [1 + k^{-1} f_1^{(1)} + k^{-2} f_2^{(1)} + \dots] \\ y_2(z) &\sim y_2^0 [1 + k^{-1} f_1^{(2)} + k^{-2} f_2^{(2)} + \dots]\end{aligned}\tag{2.90}$$

with

$$f_1^{(1)}(-z) = f_1^{(2)}(z)\tag{2.91}$$

From the discussion in section 2.7, it also follows that all f_i 's are of the form

$$f_i^{(1,2)}(z) = \sum_{j=2}^{2i} \frac{b_j^{(i)} \pm a_j^{(i)} \sin z}{\cos^j z}\tag{2.92}$$

From (2.79) and the explicit forms of χ , ζ'/ζ , ζ''/ζ and using I_n and L_n , one can see that only even j -terms exist. Now I substitute iz , using

$$\begin{aligned}\cos iz &= \cosh z \\ \sin iz &= i \sinh z\end{aligned}$$

⁹There are other methods for obtaining the α_i 's; McLachlan[16] refers (refs 92 and 93 in his book) to Ince for an alternative method.

¹⁰Note that a logarithmic term would make this procedure ill-defined.

into (2.90), giving

$$\begin{aligned} Y_1(z) &\sim Y_1^0[1 + k^{-1}F_1^{(1)} + k^{-2}F_2^{(1)} + \dots] \\ Y_2(z) &\sim Y_2^0[1 + k^{-1}F_1^{(2)} + k^{-2}F_2^{(2)} + \dots] \end{aligned} \quad (2.93)$$

where

$$F_i^{(1,2)}(z) = \sum_{j=2}^{2i} \frac{b_j^{(i)} \pm a_j^{(i)} i \sinh z}{\cosh^j z} \quad (2.94)$$

so now $F_i^{(2)} = (F_i^{(1)})^*$ and $Y_2 = Y_1^*$, which can also be derived from (2.91) and the fact that the f_i are real. The expressions for Ce_m and Se_m are then obtained by imposing the symmetry around $z = 0$, giving:

$$\begin{aligned} Ce(z) &= Y_1(z) + Y_2(z) = 2 \operatorname{Re}(Y_1(z)) \\ Se(z) &= Y_1(z) - Y_2(z) = 2i \operatorname{Im}(Y_1(z)) \end{aligned} \quad (2.95)$$

I now wish to rewrite Y in the form

$$Y(z) = R(z) \exp(i\Phi(z, k)) \quad (2.96)$$

where I included the k -dependence of Φ explicitly, because the eigenvalues k are now given by the solutions of $\operatorname{Re}(Y_1(z_b)) = 0$ or $\operatorname{Im}(Y_1(z_b)) = 0$, so by

$$\begin{aligned} \cos \Phi(z_b, k) &= 0 && \text{for } Ce\text{-type states (+)} \\ \sin \Phi(z_b, k) &= 0 && \text{for } Se\text{-type states (-)} \end{aligned}$$

or, more explicitly

$$\Phi(z_b, k) = (r + \gamma)\pi \quad (2.97)$$

where r is integral, $\gamma = 0$ for Se -type states and $\gamma = \frac{1}{2}$ for Ce -type states. The phase Φ , found from

$$A + Bi = \sqrt{A^2 + B^2} \exp \left[i \arctan \frac{B}{A} \right] \quad (2.98)$$

is not unique, since one may always add a multiple of π to it¹¹ but this does not influence (2.97), since there it just causes a shift of 1 in r .

First I rewrite Y_1^0 to the form (2.96)

$$\begin{aligned} Y_1^0(z) &= \frac{e^{2ki \sinh z}}{\cosh^m z} \left[\cosh \frac{z}{2} - i \sinh \frac{z}{2} \right]^{2m+1} \\ &= \frac{e^{2ki \sinh z}}{\cosh^m z} \left[2 \cosh^2 \frac{z}{2} - 1 \right]^{m+\frac{1}{2}} \exp \left[-i(2m+1) \arctan \tanh \frac{z}{2} \right] \\ &= \frac{\left[2 \cosh^2 \frac{z}{2} - 1 \right]^{m+\frac{1}{2}}}{\cosh^m z} \exp \left[i \left(2k \sinh z - (2m+1) \arctan \tanh \frac{z}{2} \right) \right] \end{aligned} \quad (2.99)$$

¹¹ $R(z)$ is allowed to change sign

furthermore

$$[1 + k^{-1}F_1(z) + k^{-2}F_2(z) + \dots] = \left[1 + \sum_{j=2}^{\infty} \frac{\beta^j(k) + i\alpha^j(k) \sinh z}{\cosh^j z}\right]$$

where

$$\begin{aligned}\beta^j(k) &= \sum_{i=j/2}^{\infty} k^{-i} b_j^{(i)} \\ \alpha^j(k) &= \sum_{i=j/2}^{\infty} k^{-i} a_j^{(i)}\end{aligned}$$

Now I denote

$$\begin{aligned}B(z, k) &= \sum_{j=2}^{\infty} \beta^j(k) \cosh^{-j} z \\ A(z, k) &= \sum_{j=2}^{\infty} \alpha^j(k) \sinh z \cosh^{-j} z\end{aligned}\quad (2.100)$$

then

$$[1 + k^{-1}F_1(z) + k^{-2}F_2(z) + \dots] = \sqrt{(1+B)^2 + A^2} \exp\left[i \arctan \frac{A}{1+B}\right] \quad (2.101)$$

Adding the phases of (2.99) and (2.101) gives me the total phase, which at $z = z_b$, where the ellipse has eccentricity $\epsilon = 1/\cosh z_b$, equals

$$\begin{aligned}\Phi(z_b) &\sim 2k \sinh z_b - (2m+1) \arctan \tanh \frac{z_b}{2} + \arctan \frac{A(z_b, k)}{1+B(z_b, k)} \\ &= 2k \frac{\sqrt{1-\epsilon^2}}{\epsilon} - m_1 \arctan \sqrt{\frac{1-\epsilon}{1+\epsilon}} \\ &\quad + \arctan \left[\frac{\sqrt{1-\epsilon^2}}{\epsilon} \frac{\sum_i \sum_j a_j^{(i)} \epsilon^j k^{-i}}{1 + \sum_i \sum_j b_j^{(i)} \epsilon^j k^{-i}} \right]\end{aligned}\quad (2.102)$$

The equation that determines k thus becomes

$$\begin{aligned}\frac{2\sqrt{1-\epsilon^2}}{\epsilon} k &= m_1 \arctan \sqrt{\frac{1-\epsilon}{1+\epsilon}} + (r+\gamma)\pi \\ &\quad - \arctan \left[\frac{\sqrt{1-\epsilon^2}}{\epsilon} \frac{\sum_i \sum_j a_j^{(i)} \epsilon^j k^{-i}}{1 + \sum_i \sum_j b_j^{(i)} \epsilon^j k^{-i}} \right]\end{aligned}\quad (2.103)$$

A *zeroth order formula* for k is then easily found by summing over i and j up to zeroth order, which means no summation at all: the last term in (2.103) vanishes, and I get

$$\frac{2\sqrt{1-\epsilon^2}}{\epsilon} k = m_1 \arctan \sqrt{\frac{1-\epsilon}{1+\epsilon}} + (r+\gamma)\pi + \mathcal{O}(k^{-1}) \quad (2.104)$$

These energy levels are equivalent, after unfolding, to those of a two-dimension harmonic oscillator, which is discussed by Berry and Howls[5], and can give 'strange' behavior: peaks occur that were not predictable from the fact that the system is integrable. It is therefore necessary to improve the approximation. For the first order correction, I need to sum over i and j up to the terms $1/k$. From (2.88) I see

$$\begin{aligned} b_2^{(1)} &= \frac{2m+1}{8} \\ a_2^{(1)} &= -\frac{m^2+m+1}{8} \end{aligned}$$

So

$$\frac{\sqrt{1-\epsilon^2}}{\epsilon} \frac{\sum_i \sum_j a_j^{(i)} \epsilon^j k^{-i}}{1 + \sum_i \sum_j b_j^{(i)} \epsilon^j k^{-i}} = -\frac{\sqrt{1-\epsilon^2}(m^2+m+1)\epsilon}{(2m+1)\epsilon^2+8k} + \mathcal{O}(k^{-2})$$

Inserting this into (2.103) gives me a transcendental equation for k .

Let me make the following definitions

- $\mu = \frac{1}{\epsilon\sqrt{1-\epsilon^2}}$
- $\alpha' = \frac{\epsilon}{2\sqrt{1-\epsilon^2}} = \frac{\epsilon^2\mu}{2}$
- $\beta = \alpha' \arctan \sqrt{\frac{1-\epsilon}{1+\epsilon}}$

then the *equation up to first order* becomes

$$k = m_1\beta + (r + \gamma)\pi\alpha' + \alpha' \arctan \left[\frac{1}{4\mu} \frac{m_1^2 + 3}{8k + \epsilon^2 m_1} \right] + \mathcal{O}(k^{-2}) \quad (2.105)$$

The values that γ and m_1 take are different for the different classes. They can be summarized as

- $(+, g)/ce_{2n}; \gamma = \frac{1}{2}; m_1 = 1, 5, 9, 13, 17 \dots$
- $(+, u)/ce_{2n+1}; \gamma = \frac{1}{2}; m_1 = 3, 7, 11, 15, 19 \dots$
- $(-, g)/se_{2n+1}; \gamma = 1; m_1 = 1, 5, 9, 13, 17 \dots$
- $(-, u)/se_{2n+2}; \gamma = 1; m_1 = 3, 7, 11, 15, 19 \dots$

furthermore, $r > 0$. Note that the zeroth order approximation is at most $\pi\alpha' = \frac{\pi\epsilon}{2\sqrt{1-\epsilon^2}}$ off from the real value. The order of this error only diminishes *relatively* for high k -values, not *absolutely*. Therefore, it is not good enough to determine the level spacing from. The first order approximation is off by an error of order k^{-2} , which diminishes absolutely.

2.3.4 Level Crossing

In this section I will show why the levels of the elliptical billiard cross in the asymptotic region, where the eigenvalues are given by (2.103). Note that to investigate level crossing, there is no need to compute E from k . First I look at the zeroth order eigenvalues, given by (2.104). These form a set of lines in the (ϵ, k) plane, one line for every pair (r, m_1) . Since lines with equal m_1 run parallel, they will never cross. Lines with different m_1 *will* cross, since they have different directions and are continuous. The correction term in (2.103) is seen to be at most $\pi\frac{\epsilon}{2\sqrt{1-\epsilon^2}}$. Now I focus on two lines that intersect in zeroth order. They are determined by two (independent) versions of (2.103), one for the one pair of (r, m_1) , the other for another pair. Now turn to figure 17, in which the zeroth order lines are depicted, as well as the maximal deviation from them. If the lines remain *continuous* when *all orders* are taken in account, then they have to intersect in some point in the area bounded by the dashed lines. The question is why they should remain is answered by the implicit function theorem 2.1, which in this case means that if $\frac{\partial f}{\partial k}(k, \epsilon)$ is invertible for all ϵ , then $k(\epsilon)$ is a (unique) continuous function of ϵ . For every pair (m_1, r) I will thus get a continuous lines in the (ϵ, k) -plane, if the derivative of f with respect to k

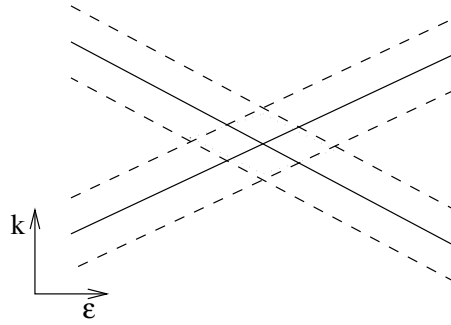


Figure 17: Two approaching levels

exists and is non-zero. I will check this for the first order correction term given in (2.105). Defining

$$t = \frac{8k + \epsilon^2 m_1}{m_1^2 + 3} 4\mu$$

Then the equation determining k or t takes on the form

$$\arctan t + \frac{m_2}{8\mu\alpha'} t + D \equiv f(t) = 0$$

where D is independent on t , and therefore not contained in the derivative to t . The derivative of the arctan is always positive, so $\frac{\partial f}{\partial t} > 0$ for all t , and it never becomes zero. Thus the solution is continuous and crossing is *inevitable*.

The equation (2.105) can be solved iteratively on a computer. I did that and displayed the lines in the (ϵ, E) plane in figure 19 of section 2.3.6, in which more numerical results are given. The asymptotic expression also sheds some light upon the independence of \mathcal{H} and \mathcal{L}^2 . Degeneracies occur when $\frac{4\beta}{\alpha'\pi}$ is rational, according to the zeroth order approximation. The values of ϵ for which this is so form a dense subset of $[0, 1]$. Thus, physically one cannot distinguish between a value of ϵ at which degeneracies occur, and a value at which they don't occur. This is still true when higher order terms are included, since I just saw that these can only shift the degeneracies by a finite amount. At a degeneracy, the value of E cannot be found from the value of λ , so \mathcal{H} and \mathcal{L}^2 are independent. It cannot be distinguish physically whether the value of ϵ is such that there are no degeneracies, so physically, one should say that \mathcal{L}^2 and \mathcal{H} are always independent quantities.

2.3.5 Unfolding

To do the required statistics, it is necessary to unfold the spectrum. This could be done using Weyl's law, but for the asymptotic formula, there is another way of getting a smooth $\bar{N}(E)$, by using the zeroth approximation of (2.104):

$$\begin{aligned} N_1(k) &= \sum_{r=1}^{\infty} \sum_{m_1=1,5,9,..}^{\infty} \Theta(k - m_1\beta - (r + \gamma)\pi\alpha') \\ N_3(k) &= \sum_{r=1}^{\infty} \sum_{m_1=3,7,11,..}^{\infty} \Theta(k - m_1\beta - (r + \gamma)\pi\alpha') \end{aligned} \quad (2.106)$$

N_3 applies to Ce_{2n+1} and Se_{2n+2} , N_1 to Ce_{2n} and Se_{2n+1} states. I will concentrate on N_1 , since from

$$N_3(k) = N_1(k - 2\beta)$$

one can get N_3 . I choose a convenient variable w :

$$\begin{aligned} w &= \frac{k - \gamma\pi\alpha' + 2\beta}{\pi\alpha'} - \frac{1}{2} \\ k &= \pi\alpha'(w + \frac{1}{2}) + \gamma\pi\alpha' - 2\beta \end{aligned} \quad (2.107)$$

then

$$\begin{aligned} N(w) &\equiv N(k) \\ &= \sum_{r=0}^{\infty} \sum_{n=0}^{\infty} \Theta(w - \frac{1}{2} - \frac{1}{2}\alpha'' - n\alpha'' - r) \end{aligned} \quad (2.108)$$

where I've defined¹²

$$\alpha'' = \frac{4\beta}{\pi\alpha'}$$

Now I use a representation of the Θ function:

$$\Theta(t) = \lim_{\eta \downarrow 0} \frac{-1}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{-i(q+i\eta)t}}{q+i\eta} dq \quad (2.109)$$

Which is a kind of Fourier representation. The η pushes the poles into the lower half plane, making the integral well-defined. To keep it well defined when the sum is taken, I have to include the same η into the exponent. Baring this in mind, I can now leave out the η , and write

$$N(w) = \frac{-1}{2\pi i} \int_{-\infty}^{\infty} \sum_{r=0}^{\infty} \sum_{n=0}^{\infty} \frac{e^{-iq(w - \frac{1}{2} - \frac{1}{2}\alpha'' - n\alpha'' - r)}}{q} dq$$

These are just geometric sums, so

$$\begin{aligned} N(w) &= \frac{-1}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{-iq(w - \frac{1}{2} - \frac{1}{2}\alpha'')}}{q} \frac{1}{1 - e^{iq}} \frac{1}{1 - e^{iq\alpha''}} dq \\ &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{-iqw}}{4q \sin(\frac{q}{2}) \sin(\frac{\alpha''q}{2})} dq \end{aligned} \quad (2.110)$$

The integral has poles on the real axis at $q = 0$, $q = 2\pi j$ and $q = \frac{2\pi l}{\alpha''}$. These actually lie in the lower half of the complex plane, due to η . The integral vanishes for $q \rightarrow -i\infty$, so the integration-path can be closed along a half circle in the lower half plane. The poles are all in the enclosed area, so $N(w)$ reduces

¹²Note that I've actually rewritten the problem to a two dimensional anisotropic harmonic oscillator, including the ground-state energy, with α'' the ratio of the frequencies

to the sum of the residues at these poles. If α'' is irrational, all poles are simple except $q = 0$, so ¹³

$$\begin{aligned} N(w) &= -\text{Res}_{q=0} \left(\frac{e^{-iqw}}{4q \sin(\frac{q}{2}) \sin(\frac{\alpha''q}{2})} \right) - \sum_{j=-\infty, j \neq 0}^{\infty} \left\{ \frac{e^{-2\pi jwi}}{4\pi j \sin(\alpha''\pi j)} + \frac{e^{-2\pi jwi/\alpha''}}{4\pi j \sin(\pi j/\alpha'')} \right\} \\ &= -\text{Res}_{q=0} \left(\frac{e^{-iqw}}{4q \sin(\frac{q}{2}) \sin(\frac{\alpha''q}{2})} \right) - \sum_{j=1}^{\infty} \frac{1}{2\pi j} \left\{ \frac{\cos(2\pi jwi)}{\sin(\alpha''\pi j)} + \frac{\cos(2\pi jwi/\alpha'')}{\sin(\pi j/\alpha'')} \right\} \end{aligned}$$

The path of integration has a negative orientation (clockwise), hence the minus-sign. I still have to calculate the first term. For small q one has

$$\begin{aligned} -e^{-iqw} &\approx -1 + iqw + \frac{1}{2}q^2w^2 + \mathcal{O}(q^3) \\ 4q \sin(\frac{q}{2}) \sin(\frac{\alpha''q}{2}) &\approx \alpha''q^3 \left[1 - \frac{1}{6}(1 + \alpha''^2) \frac{q^2}{4} \right] + \mathcal{O}(q^7) \\ \left[4q \sin(\frac{q}{2}) \sin(\frac{\alpha''q}{2}) \right]^{-1} &\approx \frac{1}{\alpha''q^3} \left[1 + \frac{1}{6}(1 + \alpha''^2) \frac{q^2}{4} \right] + \mathcal{O}(1) \end{aligned}$$

so

$$\frac{-e^{-iqw}}{4q \sin(\frac{q}{2}) \sin(\frac{\alpha''q}{2})} \approx \frac{1}{\alpha''q^3} \left[-1 + iqw + \frac{1}{2}w^2q^2 - \frac{1}{6}(1 + \alpha''^2) \frac{q^2}{4} \right] + \mathcal{O}(1)$$

and the residue is

$$-\text{Res}_{q=0} \left(\frac{e^{-iqw}}{4q \sin(\frac{q}{2}) \sin(\frac{\alpha''q}{2})} \right) = \frac{1}{2\alpha''} \left(w^2 - \frac{1 + \alpha''^2}{12} \right) \quad (2.111)$$

so finally

$$N(w) = \frac{1}{2\alpha''} \left(w^2 - \frac{1 + \alpha''^2}{12} \right) - \sum_{j=1}^{\infty} \frac{1}{2\pi j} \left\{ \frac{\cos(2\pi jwi)}{\sin(\alpha''\pi j)} + \frac{\cos(2\pi jwi/\alpha'')}{\sin(\pi j/\alpha'')} \right\} \quad (2.112)$$

The sum is not well defined. One can see that since α'' is irrational, the denominators can get arbitrarily small, so the term diverge. The first part however is supposed to be a smooth approximation to $N(w)$, so it should coincide with Weyl's law. It could then be used for unfolding. I will check this only for the quadratic term. Since

$$\begin{aligned} N_1(k) &\sim \frac{1}{2\alpha''} \left(\frac{k}{\pi\alpha'} \right)^2 = \frac{k^2}{8\pi\alpha'\beta} \\ \bar{N}(k) &\sim \frac{A}{4\pi} \frac{2m}{\hbar^2} \left[\frac{2\hbar^2 k^2}{mf^2} \right] = \frac{k^2}{8\epsilon\alpha'} \end{aligned}$$

I wondered whether $\frac{\pi\beta}{\epsilon}$ was unity. From the explicit form, it is clear that this quotient is a function of the eccentricity. The two estimates for the number of states below a given energy E are not the same. However, their numerical values do not differ much, as is seen from figure 18: the quotient is between 0.75 and 1.25. I will use the asymptotic estimate N_1 since it is more natural to the asymptotic eigenvalues, to unfold spectra found with the asymptotic method.

¹³ $q/\sin(q) \rightarrow 1$ for $q \rightarrow 0$

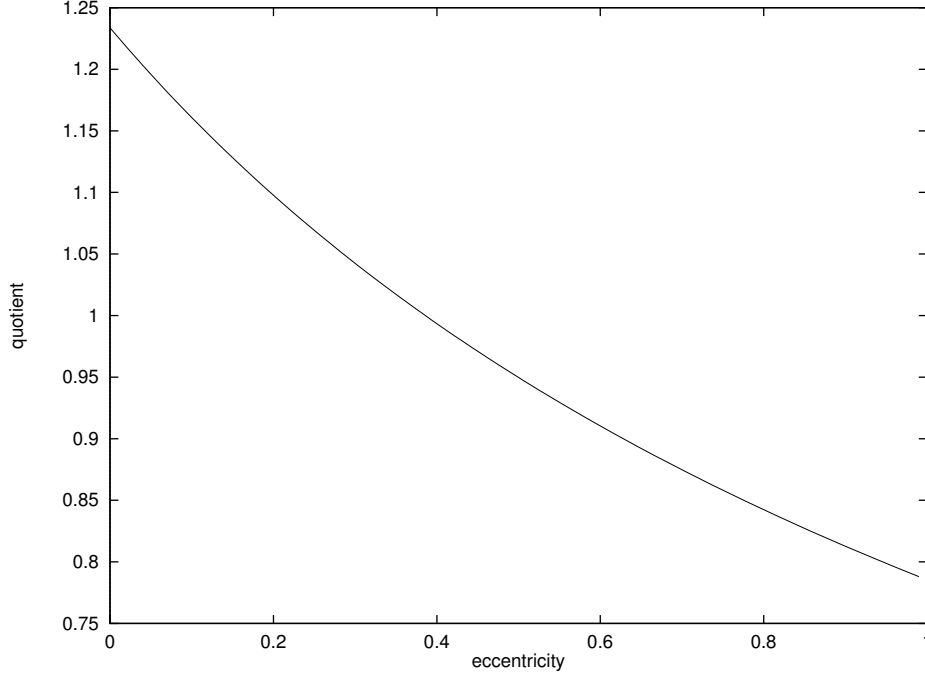


Figure 18: Quotient of the number of states according to Weyl resp. asymptotically.

2.3.6 Numerical calculations

Equation (2.105) can be solved numerically for every pair (r, m_1) . The solution lies between $m_1\beta + (r + \gamma)\pi\alpha'$ and $m_1\beta + (r + \gamma + 1)\pi\alpha'$. It is possible to get the solution of equation (2.105) by iteration. Using that $\arctan t + \arctan \frac{1}{t} = \frac{\pi}{2}$, and defining

$$\begin{aligned}\tilde{k}\alpha' &= k + \frac{\epsilon^2 m_1}{8} \\ \tilde{k}_0\alpha' &= m_1\beta + \frac{\epsilon^2 m_1}{8} + (r + \gamma + \frac{1}{2})\pi\alpha' \\ \tau &= 32 \frac{\mu\alpha'}{m_1^2 + 3}\end{aligned}$$

(2.105) becomes $\tilde{k} = \tilde{k}_0 + \arctan(\tau\tilde{k})$. I know an approximate solution to this is \tilde{k}_0 , and the deviation $\tilde{d}k = \tilde{k} - \tilde{k}_0$ obeys

$$\tilde{d}k = -\arctan\left[\tau\left(\tilde{k}_0 + \tilde{d}k\right)\right] \quad (2.113)$$

This equation is solved using the system:

$$\tilde{d}k_{i+1} = -\arctan\left[\tau\left(\tilde{k}_0 + \tilde{d}k_i\right)\right] \quad (2.114)$$

Clearly, $\tilde{d}k$ is a fixed point of this system. If it is an attractive point, then starting from the approximate solution $\tilde{d}k = 0$, one can get a better approximation by applying the transformation in (2.114), until the required accuracy is

reached. Whether or not $\tilde{d}k$ is an attractor of (2.114) depends on the derivative of the transformation at the fixed point: if its absolute value is smaller than one, the point is an attractor. The derivative is

$$\frac{-\tau}{1 + [\tau(\tilde{k}_0 + \tilde{d}k)]^2}$$

Now $\tilde{k}_0 + \tilde{d}k = \tilde{k}$, the eigenvalue to be calculated. The absolute value of the derivative is smaller than one for

$$\tilde{k} > \frac{\sqrt{\tau - 1}}{\tau} \quad (2.115)$$

and one sees that for sufficiently large \tilde{k} this is a good method of finding the solution. If \tilde{k} is known, k can be found from

$$k = -\frac{\epsilon^2 m_1}{8} + \alpha' \tilde{k} \quad (2.116)$$

The eigenvalues I find in this manner, are unfolded using (2.112). This is repeated for a large number of eigenvalues, for quite a lot of values for ϵ in some range for eigenstates of the $(-, g)$ -type. For every eigenvalue, I used (2.115) to check if the method was justifiable. This was the case for all eigenvalues that I calculated.

In figure 19, I depicted about eleven levels above the 5010th level, as a function of the eccentricity. There are too many levels and crossings to display much larger regions than $[0.5125, 0.5170] \times [5010, 5020]$, but this region is typical for all regions. I see that all levels cross.

Once I have an unfolded spectrum E'_i , I can calculate $I(s) = \int_0^s P(s') ds'$ as follows. First I sort the unfolded spectrum so I can calculate the level spacings $s_i = E_{i+1} - E_i$. These level spacings are again sorted, so $s_i \leq s_{i+1}$. If I have enough levels, say N , then the number of level spacings below a given level spacing s should be approximately $(N - 1)I(s)$. So $(s_i, \frac{i}{N-1})$ should be points of the graph of $I(s)$. From these points, I can get an estimate of $P(s)$, the derivative of $I(s)$, by calculating $\frac{I(s+ds) - I(s)}{ds}$ for not too small ds . I did this for eccentricities 0.25, 0.40, 0.50, 0.65, 0.80 and 0.95 in figure 20 to 25, in which I used the energy levels between the 5000th level and the 15000th level.

$\bar{\Delta}_3$ can also be calculated from the spectrum, using the definitions from appendix B.5. This is done for eccentricities 0.25, 0.40, 0.65, 0.80 and 0.95, depicted in figure 26 and for 0.50 in figure 27. The one in 27 has a saturation value much larger than the others, which is why I put it in an separate picture, so that the other graphs would still be distinguishable.

The graphs show the right behavior for integrable systems (see appendix B.5): they generically have a point where the slope suddenly decreases, and they show saturation.

At some values of the eccentricity, the graphs do not look like those of regular systems. This is the case, e.g., when the eccentricity equals 0.5. The zeroth order spectrum then has a lot of degeneracies and apparently the first order

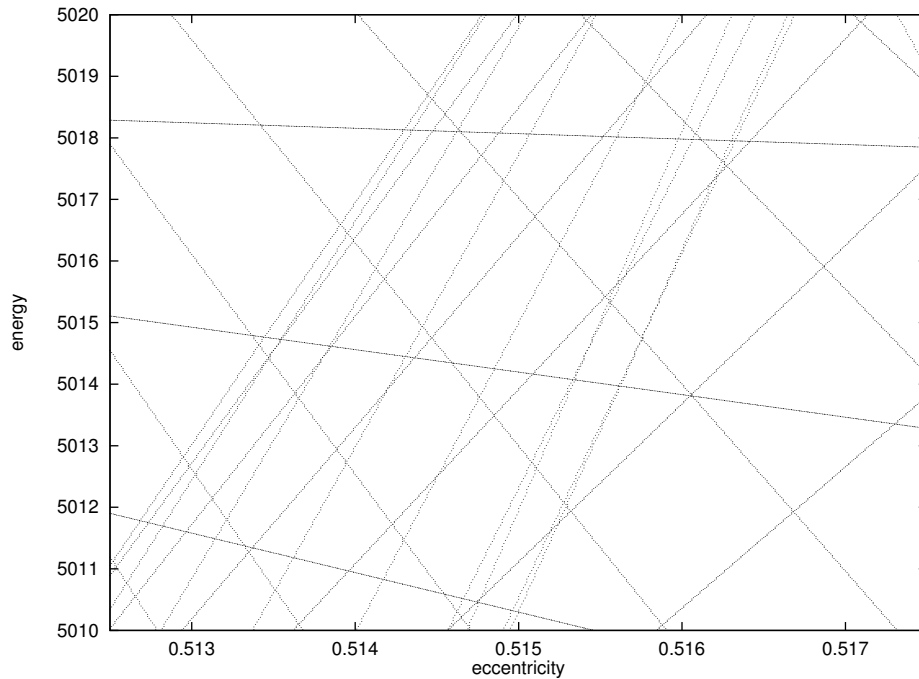
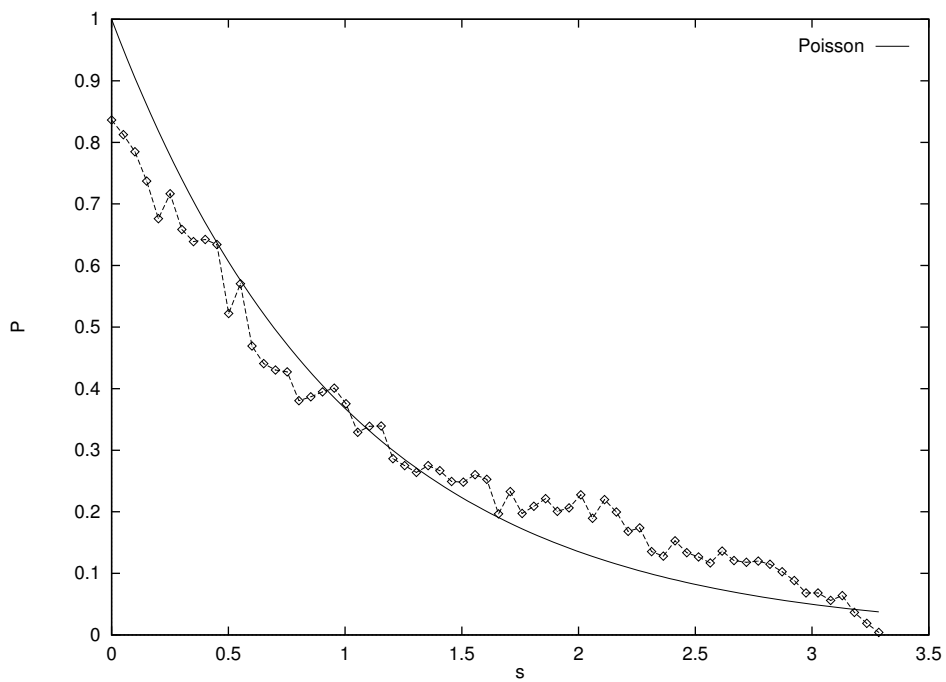
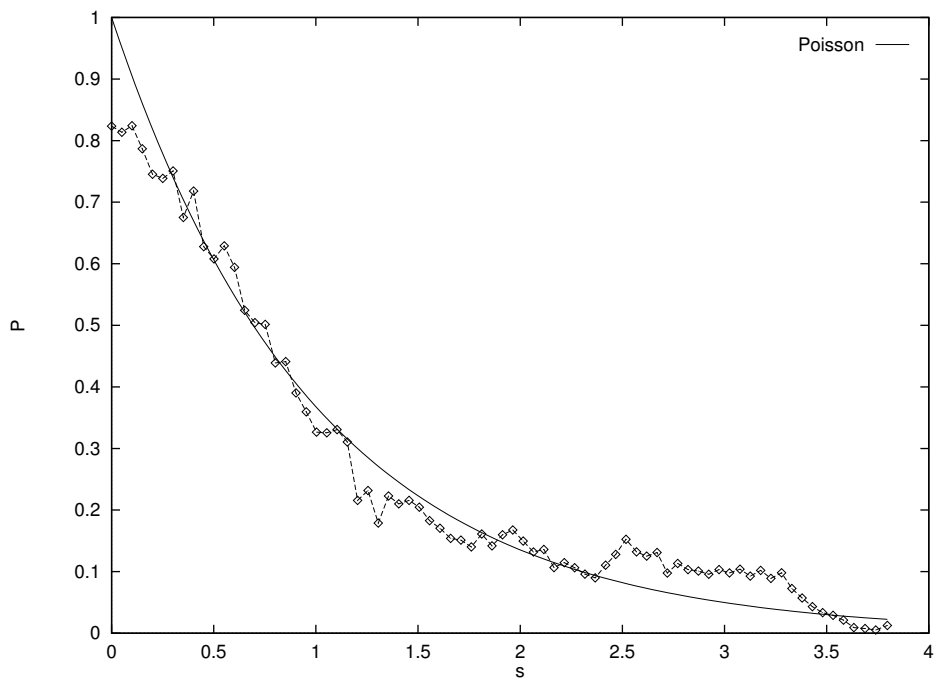
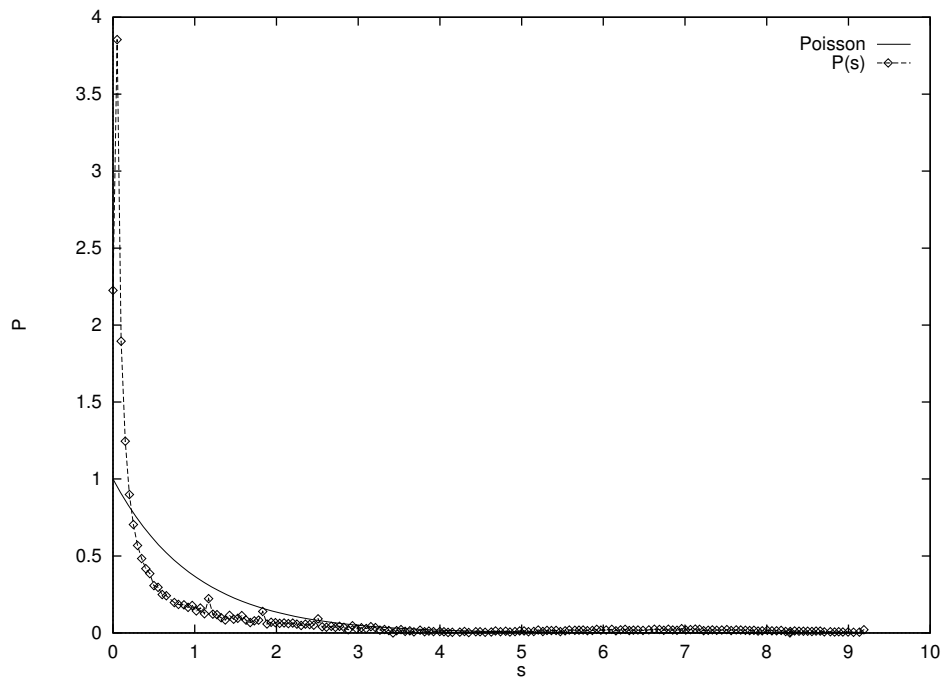
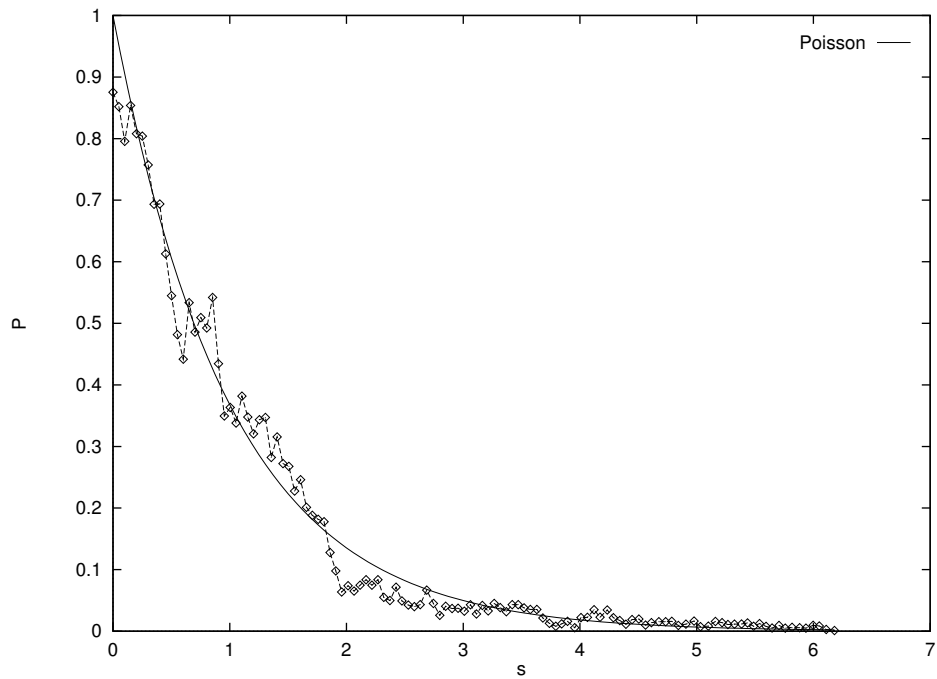


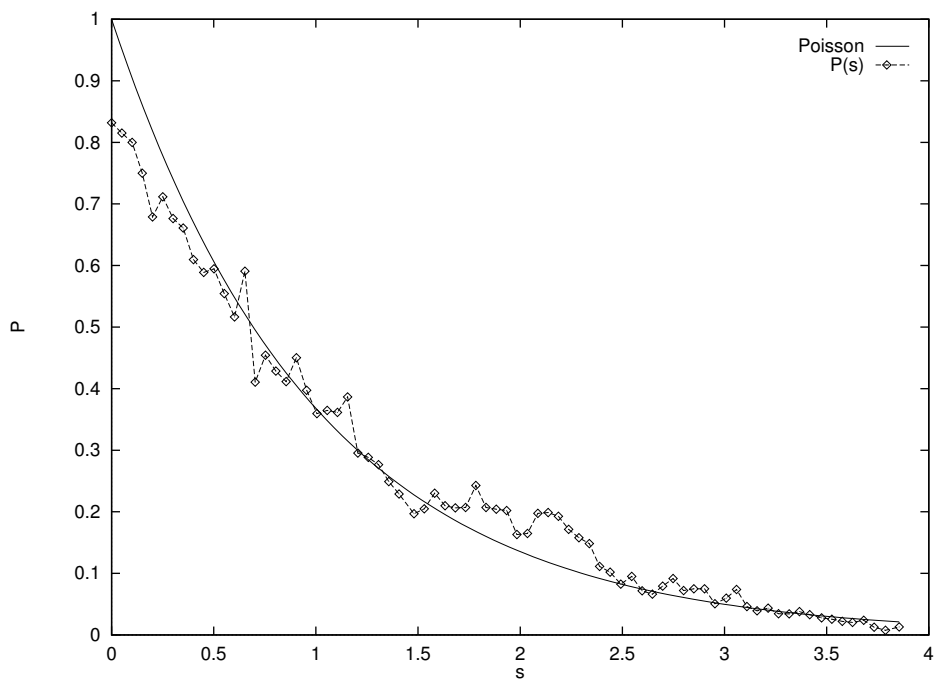
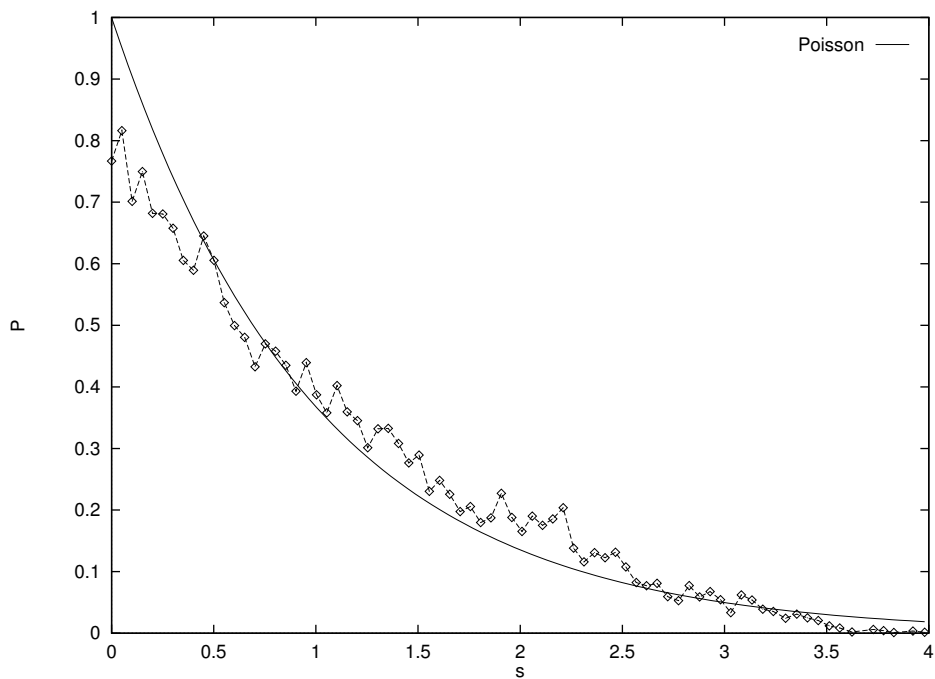
Figure 19: Energy levels (unfolded) as a function of eccentricity

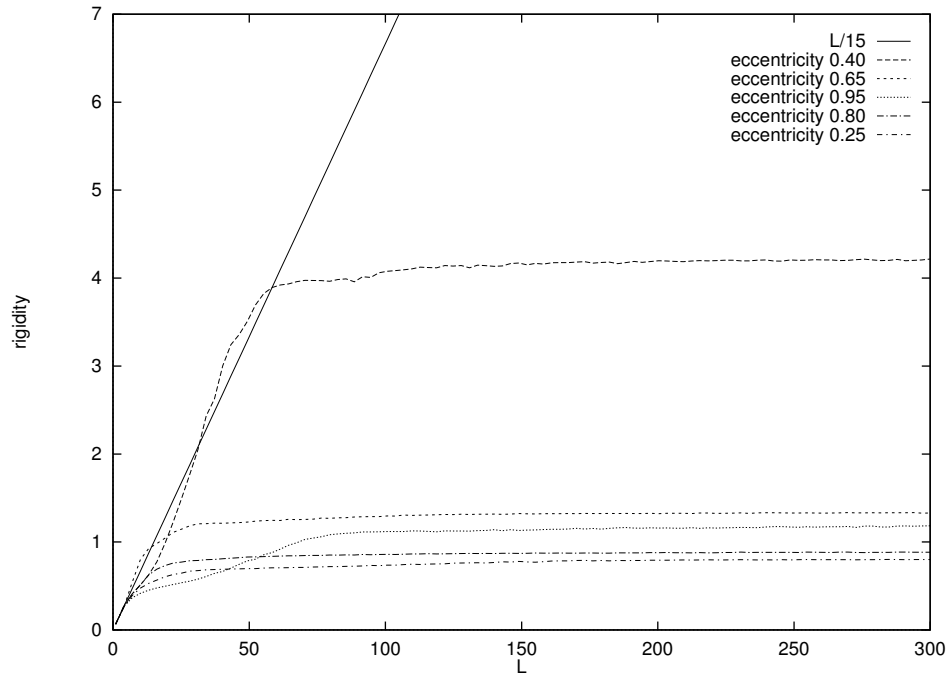
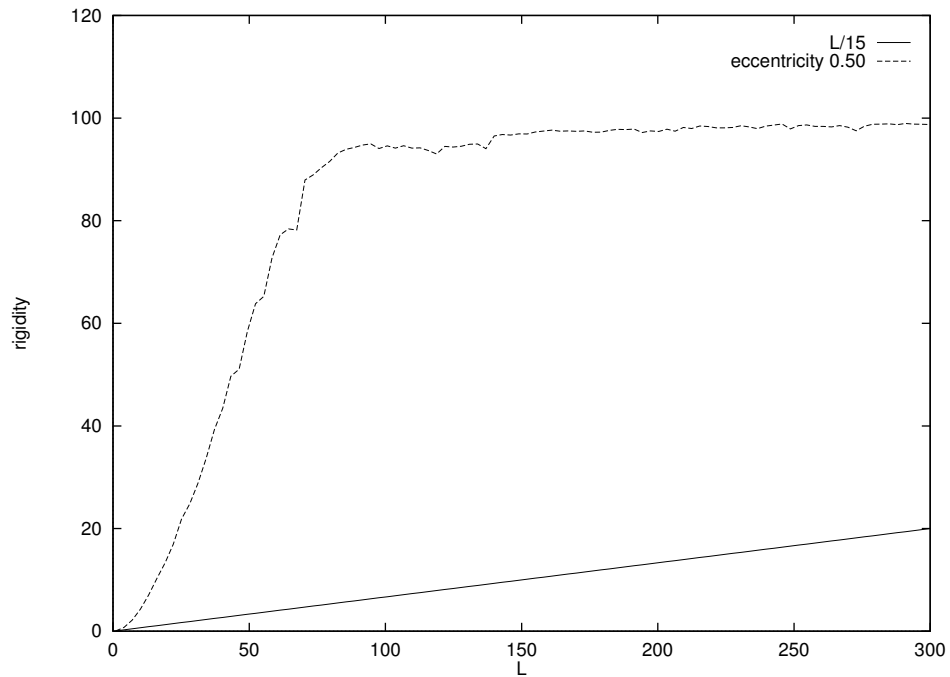
correction term cannot totally compensate. This results in a sharply peaked $P(s)$, with the peak at zero. In the graph of $\bar{\Delta}_3$, it results in a slope larger than $1/15$. The fact that there is saturation however is not changed. Large amounts of (near-)degeneracies are not typical for chaotic spectra either, so even though these graph look different than one would expect, they are still those of an integrable system. This all points to a regular spectrum, and confirms what I found in section 2.3.4. Now one might think that this is due to the asymptotic approach: the repulsion might occur at much smaller scales than can be reach in an asymptotic limit. For this reason, in the next sections I will look at the lower energy levels. The statements about $P(s)$ and $\bar{\Delta}_3$ are statistical, that apply only in the semi-classical limit. I will not find enough low-energy levels to calculate these.

For $\bar{\Delta}_3$, there is some truth in that it is the asymptotic approach that is responsible for the structure: it contains two numbers, m and r , so according to B.5 that already generates the right structure. Note however that it is the separability that enables the asymptotic approach. As seen in section 2.2.8, the separability already induces two quantum numbers, namely the numbers of the characteristic curves that intersect. These correspond to the number of zero's in the z resp. the θ -direction, exactly as m and r do. So the structure of $\bar{\Delta}_3$ is not due to the approach, but really to the separability of the billiard.

Figure 20: $P(s)$ at $\epsilon = 0.25$ Figure 21: $P(s)$ at $\epsilon = 0.4$

Figure 22: $P(s)$ at $\epsilon = 0.5$ Figure 23: $P(s)$ at $\epsilon = 0.65$

Figure 24: $P(s)$ at $\epsilon = 0.80$ Figure 25: $P(s)$ at $\epsilon = 0.95$

Figure 26: $\bar{\Delta}_3(L)$ Figure 27: $\bar{\Delta}_3(L)$ at $\epsilon = 0.50$

2.4 Low Energies – Diagonalization Method

2.4.1 Constructing a Finite Matrix from \mathcal{H}

The eigenvalue-problem of the Hamiltonian can be seen as a diagonalization problem of an infinite matrix. To make it fit for numerical analysis, I will have to approximate this in some way by a finite matrix. There are several ways to do this. First let me discuss a very straightforward method, namely that of discretization of the domain D . If D and its boundary are well-behaved, I could approximate it by little rectangles of size Δx and Δy (in two dimensions). The Laplace operator can be approximated by

$$\Delta\Psi(x, y) \approx \frac{\Psi(x + \Delta x, y) + \Psi(x - \Delta x, y) - 2\Psi(x, y)}{(\Delta x)^2} + \frac{\Psi(x, y + \Delta y) + \Psi(x, y - \Delta y) - 2\Psi(x, y)}{(\Delta y)^2}$$

for a grid point $\vec{x} = (x, y)$ inside D . For points near the boundary, the boundary conditions can be implemented by putting some terms in (2.117) to zero. Thus the Laplacian of Ψ at a point \vec{x} inside D depends linearly on Ψ in other points inside D . Numbering the \vec{x} s by i and notating $\Psi(\vec{x}_i) = \Psi_i$, I see that the Laplacian becomes a matrix. Other terms in the Schrödinger equation can be implemented by diagonal matrices, like $V\Psi_i = V(\vec{x}_i)\Psi_i = \sum_j V_i \delta_{ij} \Psi_j$ where $V_i = V(\vec{x}_i)$. Thus $T + V$ is approximated by a matrix M . It is expected that this finite grid method will not give the higher energies correctly, but that the lower energies get better when the matrix is enlarged (grid points get closer to each other). A version of this method in which boundary conditions can be easily implemented can be used if there exists a coordinate transformation that transforms the boundary into a rectangle. Dirichlet boundary conditions, say, can then be implemented by putting certain elements of M equal to zero.

There are other ways to convert the Schrödinger equation to an eigenvalue problem for a matrix, e.g. by *expanding* it in a Fourier sum and cut the series off at some \vec{k} value. Or more general, one can expand in a complete set of functions $|k\rangle$ on D that satisfy the boundary conditions:

$$\begin{aligned} E\Psi &= \mathcal{H}\Psi \\ \sum_k E a_k |k\rangle &= \mathcal{H} \sum_k a_k |k\rangle \\ &= \sum_k a_k \mathcal{H} |k\rangle \\ &= \sum_k a_k \sum_{k'} |k'\rangle \langle k' | \mathcal{H} | k \rangle \\ &= \sum_{k'} [\sum_k H_{k'k} a_k] |k'\rangle \end{aligned} \quad (2.117)$$

where

$$H_{k'k} = \langle k' | \mathcal{H} | k \rangle \quad (2.118)$$

Exchanging the summation indices k and k' and equating the different terms in the expansion gives

$$\sum_{k'} H_{kk'} a_{k'} = E a_k \quad (2.119)$$

If I now cut off the k values, H is a finite matrix and (2.119) is the eigenvalue problem for H . This matrix could be a better approximation, but there are some disadvantages too. The calculation of the elements of H generally requires an integration that cannot be done explicitly, and thus requires a numerical approach. Also the matrix M has only five elements per row, whereas H will most likely have more. The less elements, the less computation is needed. Nevertheless, some of the methods that take advantage of a sparse matrix (that is a matrix that has a lot of zero elements), like the Lanczos algorithm, are not very stable near degeneracies¹⁴, and above that the discretization also is very inefficient, in the sense that one can only expect about 10 percent of the eigenvalues of the finite matrix to be correct – I checked this for the rectangle. And so I will use the last method, writing the Hamiltonian on the basis of a (finite) set of basis-vectors. Having a non-sparse matrix, I have to use all entries in the matrix, which means the the memory of the computer restricts the number of basis-vectors, before time restricts it.

A particular way of constructing the matrix is used in Ayant and Arvieu [1], and I will use the same method so I can compare the results. Ayant and Arvieu were not looking at level repulsions or quantum chaos, their article investigates the effect of the three-dimensional environment that a two dimensional elliptical billiard in reality always has, and find a very large dependence of the energy levels of the billiard on the form of the environment. Their graphs of levels of the two-dimensional billiard (not in any environment, so that is the problem I'm looking at), show some repelling levels, but they could be due to computational effects, and I would like to check that. They reach a matrix of 140 by 140 element. I am limited to a matrix of 104 by 104, which is somewhat more reduced even, because of the consistent way of constructing the base, as I will show.

First, a transformation is performed to coordinates in which the ellipse is a circle:

$$\begin{aligned}x' &= \frac{R}{a}x \\y' &= \frac{R}{b}y\end{aligned}\tag{2.120}$$

where R is defined by

$$\frac{2}{R^2} = \frac{1}{a^2} + \frac{1}{b^2}\tag{2.121}$$

After this transformation the Hamiltonian reads

$$\begin{aligned}\mathcal{H}\Psi &= -\frac{\hbar}{2m}\Delta'\Psi - \frac{\hbar}{2m}\frac{b^2 - a^2}{a^2 + b^2}\left(\frac{\partial^2}{\partial x'^2} - \frac{\partial^2}{\partial y'^2}\right)\Psi \\ &= (\mathcal{H}_0 + \mathcal{H}_1)\Psi\end{aligned}\tag{2.122}$$

Now \mathcal{H}_0 is just the Hamiltonian of a circular billiard, so it makes sense to take the eigenfunctions of \mathcal{H}_0 , which are, in polar coordinates corresponding to

¹⁴For ordinary second order differential equations, there does exist a stable method: the matrix becomes tri-diagonal and the QL algorithm (explained in appendix D) can be applied.

(x', y') .

$$\Phi_{nm}(r') = \frac{1}{\sqrt{\pi}R J'_m(\zeta_{nm})} J_m(\zeta_{nm} \frac{r'}{R}) e^{im\phi'} \quad (2.123)$$

with ζ_{nm} the n th zero of the cylindrical Bessel function $J_m(\rho)$. Again, the symmetries of the ellipse – reflection with respect to $x = 0$ and $y = 0$ – should be extracted first, therefore the following combinations and sets have to be separately handled:

1. $(+, g)$ $\pi_x = +1$, $\pi_y = +1$, states are expanded in

$$\begin{aligned} |A; n0\rangle &= \Phi_{n0} \\ |A; nm\rangle &= (\Phi_{nm} + \Phi_{n-m})/\sqrt{2} \end{aligned}$$

with m even and nonnegative.

2. $(-, g)$ $\pi_x = -1$, $\pi_y = -1$, states are expanded in

$$|B; nm\rangle = (\Phi_{nm} - \Phi_{n-m})/\sqrt{2}$$

with $m > 0$ even.

3. $(+, u)$ $\pi_x = -1$, $\pi_y = +1$, states are expanded in

$$|C; nm\rangle = (\Phi_{nm} + \Phi_{n-m})/\sqrt{2}$$

with $m > 0$ odd.

4. $(-, u)$ $\pi_x = +1$, $\pi_y = -1$, states are expanded in

$$|D; nm\rangle = (\Phi_{nm} - \Phi_{n-m})/\sqrt{2}$$

with $m > 0$ odd.

It is convenient to define

$$\alpha = \frac{a^2 - b^2}{a^2 + b^2} \quad (2.124)$$

since in units of $\hbar^2/2mR^2$, the matrix elements of \mathcal{H}_1 then become

$$\langle \Phi_{n'm+2} | \mathcal{H}_1 | \Phi_{nm} \rangle = 2\alpha(m+1) \frac{\zeta_{nm}\zeta_{n'm+2}}{\zeta_{nm}^2 - \zeta_{n'm+2}^2} \quad (2.125)$$

where Ayant and Arvieu use "various recurrence relations between Bessel functions and their derivatives". For $m = -1$ and $n' = n$ this formula should be replaced by

$$\langle \Phi_{n1} | \mathcal{H}_1 | \Phi_{n-1} \rangle = \frac{1}{2} \alpha \zeta_{n1}^2 \quad (2.126)$$

Other elements can be found using the symmetry properties

$$\begin{aligned}\langle \Phi_{n'-m'} | \mathcal{H}_1 | \Phi_{n-m} \rangle &= \langle \Phi_{n'm'} | \mathcal{H}_1 | \Phi_{nm} \rangle \\ \langle \Phi_{n'-m-2} | \mathcal{H}_1 | \Phi_{n-m} \rangle &= \langle \Phi_{n-m} | \mathcal{H}_1 | \Phi_{n'-m-2} \rangle \\ &= \langle \Phi_{n'm+2} | \mathcal{H}_1 | \Phi_{nm} \rangle\end{aligned}$$

or are zero. The elements of the unperturbed \mathcal{H}_0 are, again in units of $\hbar^2/2mR^2$,

$$\langle \Phi_{n'm'} | \mathcal{H}_0 | \Phi_{nm} \rangle = \delta_{n'n} \delta_{m'm} \zeta_{nm}^2 \quad (2.127)$$

It is therefore consistent to take as a base all n and m such that the element $\langle \Phi_{nm} | \mathcal{H}_0 | \Phi_{nm} \rangle$ is smaller than some fixed energy. In [1] this energy is taken to be (square of) the first zero of J_{40} , which gives them 140 zeros. I have to restrict myself to the first zero of J_{33} , giving 98 zeros for Ce_{2n} -states. This completes the method to compute a finite \mathcal{H} .

2.4.2 Numerical Results

In the previous section I stated how a matrix can be constructed of which the lowest eigenvalues should be good approximations of the energies of the ellipse. Once this matrix is constructed, it of course has to be diagonalised. The diagonalization method used is discussed in the appendix.

The eigenvalues are determined for a lot of values of the eccentricity, running from 0 to 1. The energies of Ce_{2n} states lower than $300 \frac{\hbar^2}{2mR^2}$ are depicted in figure 28. Apparently, all the levels *cross*. To further confirm this, I zoomed in on five areas, depicted in figures 29 to 33. According to Ayant and Arvieu[1] the approaching levels in the second zoom and the last two zooms repel. No repulsion is seen in my figures, which in fact show crossing. I have to conclude that the diagonalization routine that Ayant and Arvieu used is not well behaved around degeneracies, and the repulsions they find are due to *computational errors*, like the one I modeled in section 2.1.1. In fact, the QL method I used is capable of dealing with degeneracies, as stated in the appendix.

2.4.3 Another Method

In Traiber, Fendrik, Bernath[23] a different method is used for proving [1] wrong. They obtain eigenvalues in a way which turns out to be closely related to the treatment in terms of characteristic curves in section 2.2.8¹⁵. The authors have used an algorithm ("352 from ACM library") which enables them to access the solutions of the Mathieu equation and its characteristic values numerically. Via a kind of Newton-Raphson procedure they find the eigenvalues of \mathcal{H} and \mathcal{L}^2 . Plotted against one another, it is seen that they follow the characteristic curves. The energy values are also plotted against $\frac{1}{\sqrt{1-\epsilon^2}}$, and they find the same crossings as in figure 28 as expected since they effectively use characteristic curves and according to section 2.2.8 this means that generically levels cross.

¹⁵Though the authors do not mention that.

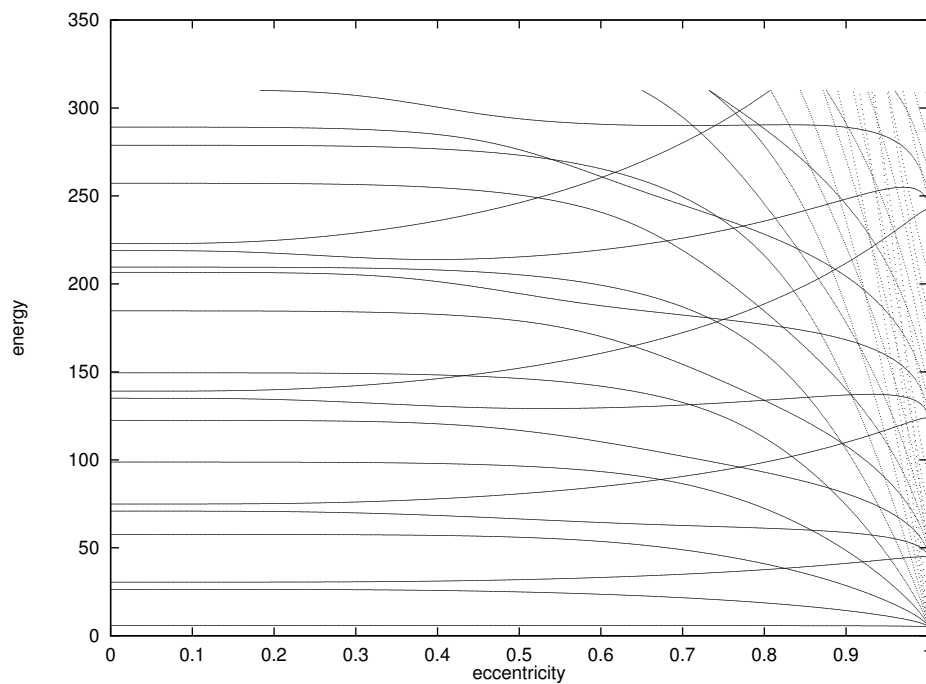


Figure 28: Eigenvalues of the Ellipse - overview

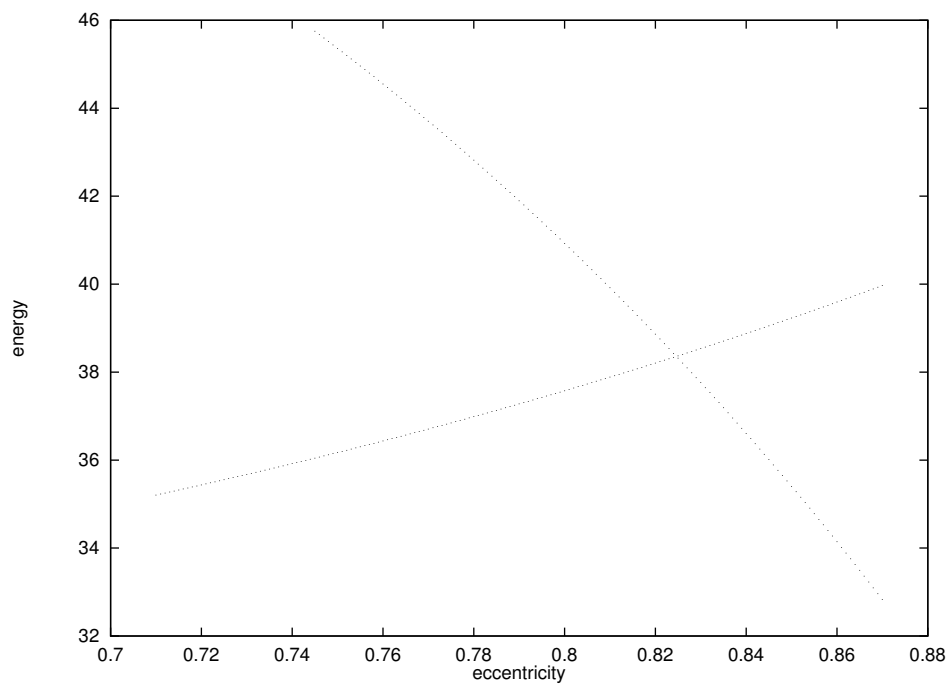


Figure 29: Eigenvalues of the Ellipse - zoom I

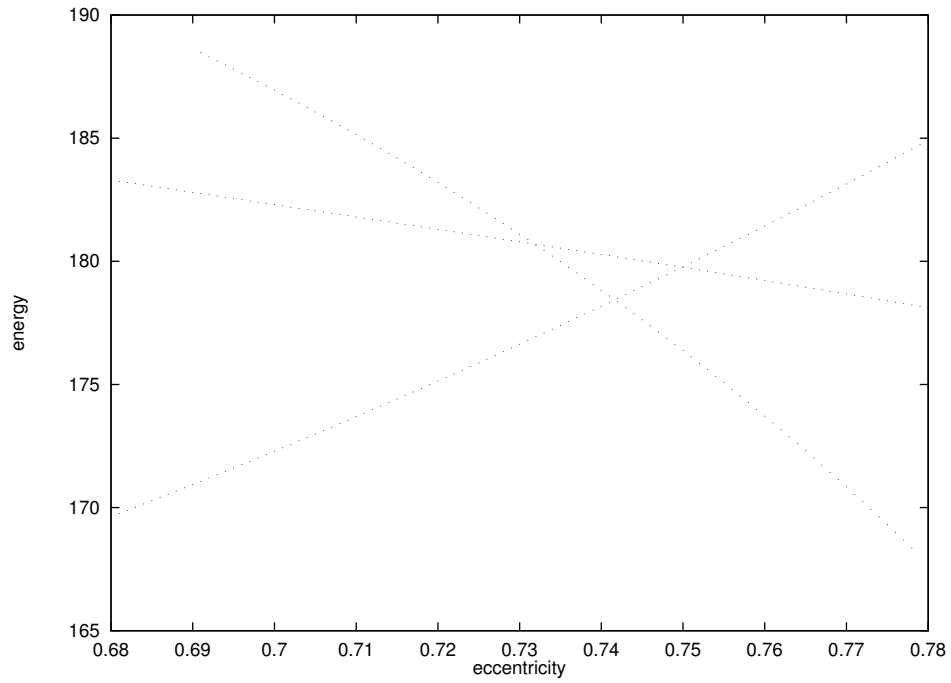


Figure 30: Eigenvalues of the Ellipse - zoom II

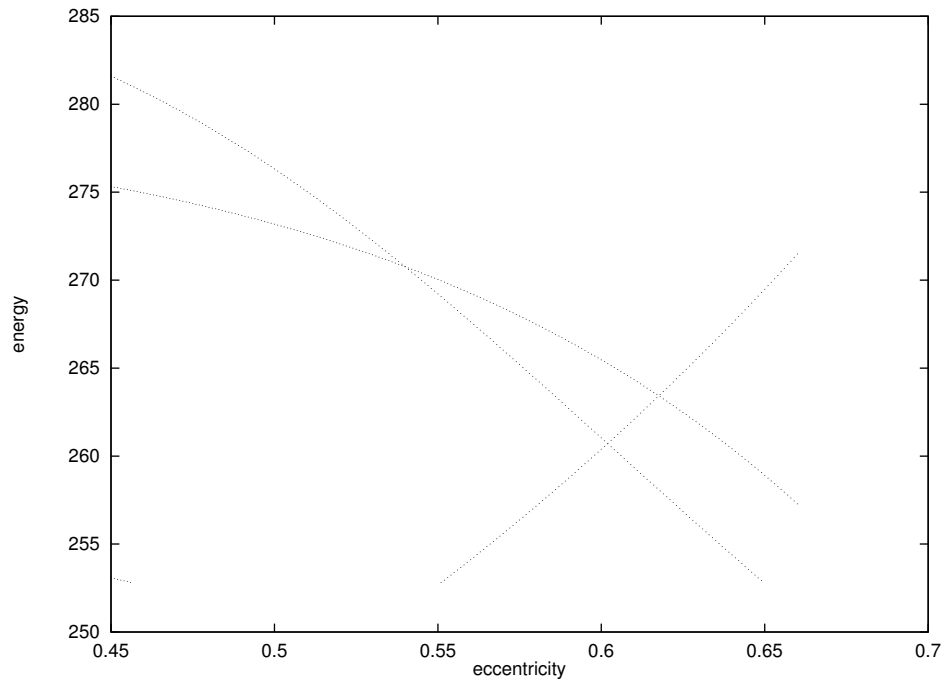


Figure 31: Eigenvalues of the Ellipse - zoom III

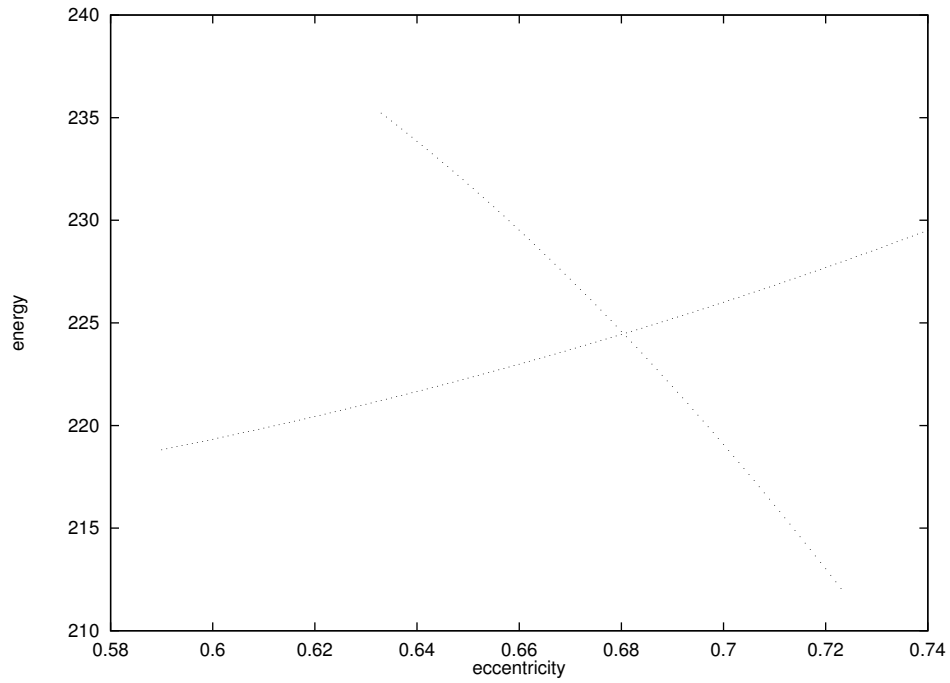


Figure 32: Eigenvalues of the Ellipse - zoom IV

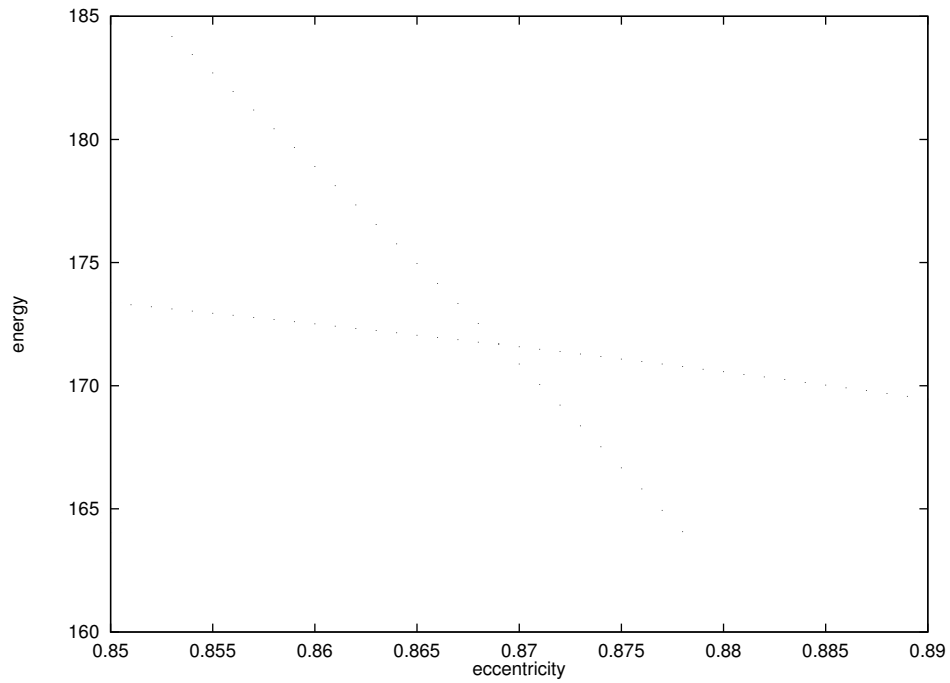


Figure 33: Eigenvalues of the Ellipse - zoom V

2.5 Summary

As in the classical case, the quantity \mathcal{L}^2 is not conserved in the sense that $[\mathcal{L}^2, \mathcal{H}] = 0$. However, again $\mathcal{L}^2 + X = Z$ is conserved. Thus one expects a regular spectrum of \mathcal{H} . The eigenvalue problems seem to be equivalent, so the question arose whether these quantities are really independent. If they aren't, maybe the spectrum could be less regular. In fact, there exists an article by Ayant and Arvieu[1], that contains a figure of the lower energy levels of the elliptical billiard as a function of the eccentricity, of which some show repulsion – a typical phenomenon for chaotic spectra. So my aim was to calculate as much levels of the spectrum as possible to do the statistic necessary to distinguish chaotic from regular spectra.

Despite the separability of the problem, it is not soluble. I could only get asymptotic results. These show level crossing, and the statistical quantities are not like chaotic ones. For most eccentricities, $P(s)$ looks like that for regular spectra. $\Delta_3(L)$ also seems to have the right structure of a regular spectrum. For some energy values, e.g. $\epsilon = 0.5$, the spectra looks a bit like a two-dimensional harmonic oscillator, as the asymptotic formula suggests. It is not clear whether this is a real effect or due to the method.

There are also theoretical reasons why levels should cross. The eigenfunctions can be represented by intersection points of two sets of characteristic curves – that do not intersect among them selfs – in the (q, a) -plane – where q and a are the eigenvalues of \mathcal{H} and \mathcal{L}^2 . When the eccentricity changes, one of these sets changes, continuously, and so will the intersection points. Two points far apart will move independently. Since the spectrum of \mathcal{H} is the projection of these points, they could be close together in the spectrum. Because of their independence, there is no reason why they should start to repel under a further change of the eccentricity, if they were initially approaching. So generically, they will cross.

Finally, I redid the numerical calculation of Ayant and Arvieu, and found the same levels as they did, except that they *crossed*. The overall picture seems to be that of a regular spectrum, with the understanding that even a regular spectrum can give strange results in certain cases.

3 Two Dimensional Separable Systems

In this part I will generalize the elliptical billiard to the class of all integrable systems in two dimensions with a conserved quantity quadratic in the momenta. First the quantum-mechanical case is considered, then the classical case is treated, giving the same result.

3.1 Quantum-Mechanical Separability

3.1.1 Construction of All Two Dimensional Separable Billiards

The elliptical billiard can be generalized to a class of problem with the same characteristics:

- It is a *separable, billiard-like* system,
- The second constant of motion \mathcal{L}^2 has an *ill-defined commutator* with the Hamiltonian \mathcal{H} , which can be fixed by adding a term X to \mathcal{L}^2 ,
- The eigenvalue problems of \mathcal{H} and \mathcal{L}^2 are *equivalent*, thus no exact solution can be found by separation.

It turns out that the first characteristic is already very restrictive, as I will show in this section. The last two are then shown to be equivalent requirements. They are also shown to be very common in the class of separable systems.

I will look at this problem from two viewpoints. The first is to look at a general separable system. The other is to look at a Hamiltonian of the form

$$\mathcal{H} = \frac{p_x^2 + p_y^2}{2m} + V(x, y)$$

in an arbitrary coordinate system. The resulting expressions for \mathcal{H} and \mathcal{L}^2 should be identical if V is of the hard-wall type, which poses a restriction on the allowed coordinate transformations, and thus on the shapes of the billiards in this class of systems.

A separable system in two dimensions is a system in which the Schrödinger equation can be written as two ordinary differential equations, each containing only one coordinate, z or θ . This is done by substituting $\Psi(z, \theta) = Y(z)T(\theta)$ and then re-ordering the Schrödinger equation such that the left hand side depends on z only and the right hand side depends on θ only. Then both sides have to equal the same constant λ . Since the energy E and the constant λ appear linearly in the equations (without differential operators), the most general form of the two separate equations is

$$\begin{aligned} D_z Y(z) + \lambda f_1(z) Y(z) + E f_2(z) Y(z) &= 0 \\ D_\theta T(\theta) + \lambda g_1(\theta) T(\theta) + E g_2(\theta) T(\theta) &= 0 \end{aligned} \quad (3.1)$$

where D_z and D_θ are differential operators of second order and f_1, f_2, g_1 and g_2 are functions of z and θ respectively. The general form for D_z and is ¹

$$D_z = \frac{\partial^2}{\partial z^2} + q(z) \frac{\partial}{\partial z} + r(z) \quad (3.2)$$

¹since any multiplicative function in front of $\frac{\partial^2}{\partial z^2}$ can be absorbed into the other functions

Now the $\frac{\partial}{\partial z}$ -term can be removed by writing

$$Y'(z) = Y(z) \exp \left[-\frac{1}{2} \int^z q(z') dz' \right]$$

This can also be viewed as a coordinate shift in the z -direction. Since such a transformation will not affect the shape of a billiard system, I can restrict myself to systems where D_z does not contain any first order derivatives. Of course the same is true for D_θ , so

$$\begin{aligned} D_z &= \frac{\partial^2}{\partial z^2} + r(z) \\ D_\theta &= \frac{\partial^2}{\partial \theta^2} + \rho(\theta) \end{aligned} \quad (3.3)$$

More simplifications can be made by one-dimensional coordinate transformations that set $f_1 = 1$ and $g_1 = 1$, but I will leave this to later. From the general form (3.1), I can reconstruct the Hamiltonian by eliminating λ . In the same way I can construct the quantity associated with λ , which I call Z , by eliminating E . I define

$$M(z, \theta) = \frac{\hbar^2}{2m} [g_2(\theta) f_1(z) - g_1(\theta) f_2(z)] \quad (3.4)$$

which is proportional to the determinant of (3.1) viewed as a linear set of equations in λ and E . The quantities become

$$\mathcal{H} = \frac{\hbar^2}{2m} \frac{g_1(\theta) D_z - f_1(z) D_\theta}{M(z, \theta)} \quad (3.5)$$

$$Z = \frac{\hbar^2}{2m} \frac{f_2(z) D_\theta - g_2(\theta) D_z}{M(z, \theta)} \quad (3.6)$$

Since the solutions of the separated problem are eigenfunctions of both \mathcal{H} and Z , these two quantities have to commute

$$[\mathcal{H}, Z] = 0 \quad (3.7)$$

In appendix C.6, some attention is given to hermiticity of the observables \mathcal{H} and Z . The last characteristic is seen to be implemented, I have two hermitian operators with equivalent separated problems².

I can split the Hamiltonian into a kinetic part and a potential part, such that

$$\begin{aligned} T &= \frac{\hbar^2}{2m} \frac{g_1(\theta) \frac{\partial^2}{\partial z^2} - f_1(z) \frac{\partial^2}{\partial \theta^2}}{M(z, \theta)} \\ V &= \frac{\hbar^2}{2m} \frac{g_1(\theta) r(z) - f_1(z) \rho(\theta)}{M(z, \theta)} \end{aligned} \quad (3.8)$$

²provided that f_1 , f_2 , g_1 and g_2 are all non-zero.

I can do the same for Z , extracting a term analogous to X . From (3.7) it is seen that $[\mathcal{H}, Z - X] = [\mathcal{H}, \mathcal{L}^2] \neq 0$, and actually it will be infinite if the potential has a discontinuity. This is fixed by again adding X .

The kinetic part reads

$$T = -\frac{\hbar^2}{2m}\Delta$$

in a new coordinate system, so

$$\Delta = \frac{-g_1(\theta)\frac{\partial^2}{\partial z^2} + f_1(z)\frac{\partial^2}{\partial \theta^2}}{M(z, \theta)} \quad (3.9)$$

The Laplacian in an arbitrary coordinate system is calculated in appendix C.2, with the result

$$\Delta = (J^T J)_{jk}^{-1} \left[\partial_j \partial_k - (\partial_j J_{mk}) J_{lm}^{-1} \partial_l \right]$$

In order that this equals (3.9), $(J^T J)^{-1}$ needs to be diagonal and $(J^T J)_{jk}^{-1}(\partial_j J_{mk})$ needs to be zero. If $(J^T J)^{-1}$ is diagonal, then so is $J^T J$. One can make them proportional to the unity matrix by appropriate scaling. So the minimal requirements are

- $J^T J$ is diagonal
- $\partial_j J_{mj} = 0$

If these are fulfilled then Δ takes the form

$$\Delta = \frac{1}{\det^2 J} [(J_{22}^2 + J_{12}^2)\partial_1^2 + (J_{21}^2 + J_{11}^2)\partial_2^2] \quad (3.10)$$

since $(J^T J)_{11} = J_{11}^2 + J_{12}^2$ and $(J^T J)_{22} = J_{22}^2 + J_{21}^2$. Comparing this with (3.9), I see that

$$g_1(\theta) = -\frac{J_{22}^2 + J_{12}^2}{\det J}$$

$$f_1(z) = \frac{J_{21}^2 + J_{11}^2}{\det J}$$

Now $\det(J^T J) = \det^2 J = (J_{22}^2 + J_{12}^2)(J_{21}^2 + J_{11}^2)$, so $g_1(\theta)f_1(z) = -1$ and the functions have to be constants. This is precisely the result of the one-dimensional coordinate transformation I mentioned before. Thus Δ becomes

$$\Delta = \frac{1}{\det J} [\partial_1^2 + \partial_2^2] \quad (3.11)$$

Since by scaling z and θ , the constant can be set to 1.³ So I can restrict myself to transformations where

$$(J^T J)_{ij} = \det J \delta_{ij} \quad (3.12)$$

³This scaling does not affect the form of a billiard.

This means that I have

$$J_{11}^2 + J_{21}^2 = J_{12}^2 + J_{22}^2 = J_{11}J_{22} - J_{12}J_{21}$$

which is a normalization requirement on the columns of J , and

$$J_{11}J_{12} + J_{22}J_{21} = 0$$

which is an orthogonality requirement. These imply that J can be written in the form

$$J = \sqrt{\det J} \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix}$$

so

$$\begin{aligned} J_{11} &= J_{22} \\ J_{12} &= -J_{21} \end{aligned}$$

These are precisely the Cauchy-Riemann equations. So the transformation can be written in the form (from here on the procedure can be found in Morse and Feshbach[18])

$$x_1 + ix_2 = f(z + i\theta) \quad (3.13)$$

Then the second requirement is now also satisfied, using (3.13), because

$$\begin{aligned} \partial_j J_{1j} &= \frac{\partial^2 x_1}{\partial z^2} + \frac{\partial^2 x_1}{\partial \theta^2} = 0 \\ \partial_j J_{2j} &= \frac{\partial^2 x_2}{\partial z^2} + \frac{\partial^2 x_2}{\partial \theta^2} = 0 \end{aligned} \quad (3.14)$$

So (2.27) holds, as does (2.28) (with $f=1$). M has to be the sum of a function of θ and a function of z . Now⁴

$$\left(\frac{\partial x_1}{\partial z}\right)^2 + \left(\frac{\partial x_1}{\partial \theta}\right)^2 = \left|\frac{df}{dw}\right|^2 = \frac{df^*}{dw^*} \frac{df}{dw}$$

where $w = z + i\theta$. Furthermore

$$\frac{\partial^2}{\partial z \partial \theta} = i \frac{\partial^2}{\partial w^2} - i \frac{\partial^2}{\partial w^{*2}}$$

So the separability condition $\frac{\partial^2 M}{\partial z \partial \theta} = 0$, becomes

$$\frac{df^*}{dw^*} \frac{d^2}{dw^2} \frac{df}{dw} = \frac{df}{dw} \frac{d^2}{dw^{*2}} \frac{df^*}{dw^{*2}} \nu$$

or

$$\left(\frac{df}{dw}\right)^{-1} \frac{d^2}{dw^2} \frac{df}{dw} = \left(\frac{df^*}{dw^*}\right)^{-1} \frac{d^2}{dw^{*2}} \frac{df^*}{dw^{*2}} = \nu \quad (3.15)$$

where ν is a constant, since both sides depend on different independent variables. This gives me a differential equations to be solved. The solution are

⁴With * I denote complex conjugation.

- $\nu = 0$: $f(w) = \alpha + \beta w + \frac{1}{2}\gamma w^2$. For $\gamma = 0$ this generates *rectangular* coordinates, otherwise this generates *parabolic* coordinates.
- $\nu = 1$: $f(w) = \frac{e^w - \alpha e^{-w}}{1 + \alpha}$. For $\alpha = 0$, this generates *polar* coordinates after the substitution $r = e^z$, otherwise one gets *elliptic* coordinates⁵. For $\alpha = 1$, I regain (1.1).

So I see that there are only four types of separable coordinate systems: rectangular, polar, parabolical and elliptical, and thus there are only four types of separable billiards. The rectangle and the circle are well-covered textbook examples. The ellipse is not so simple a problem, as I showed in the previous sections. I did not consider the parabolic billiard yet. Besides billiards I can also generate systems governed by a potential, which has to be of the form

$$V(z, \theta) = \frac{V_z(z) + V_\theta(\theta)}{M(z, \theta)}$$

A billiard can again be found by taking a infinite step function for V_z or V_θ . From these systems, all separable quantum-mechanical Hamilton systems in two dimensions can be found by performing certain coordinate transformations. In this way several of the choices of coordinate systems made in the derivation can be undone, but one keeps the conserved quantity Z .

3.2 Classical Separability

3.2.1 Separability of the Billiards

Continuing the general viewpoint of the previous section, I want to look at classical separable systems too. To do this a different approach is needed to give new insights into the matter. The new approach I will follow is that of the Hamilton-Jacobi formalism[11], which is explained in appendix A.2. In this section I will show that the systems found in section 3.1.1 are also separable classically. To do this I look at an arbitrary system with a Hamiltonian of the form

$$\mathcal{H} = \frac{|\vec{p}|^2}{2m} + V \quad (3.16)$$

Thus the time independent Hamilton-Jacobi equation for this system is

$$\left| \frac{\partial W}{\partial \vec{q}} \right|^2 + V - E = 0 \quad (3.17)$$

For the quantum-mechanical case, I will now write the wave-function as⁶

$$\Psi(\vec{q}) = e^{T + \frac{i}{\hbar} S} \quad (3.18)$$

⁵of which z is transformed.

⁶The imaginary part of the exponent can be shown to be of order \hbar^{-1} , and I denoted this explicitly.

The time-independent schrödinger equation can then be split in its real and imaginary part, which become

$$-\frac{\hbar^2}{2m} \left(\frac{\partial}{\partial \vec{q}} \cdot \frac{\partial T}{\partial \vec{q}} + \left| \frac{\partial T}{\partial \vec{q}} \right|^2 \right) + \left(\left| \frac{\partial S}{\partial \vec{q}} \right|^2 + V - E \right) = 0 \quad (3.19)$$

$$\frac{\partial}{\partial \vec{q}} \cdot \frac{\partial S}{\partial \vec{q}} + 2 \frac{\partial S}{\partial \vec{q}} \cdot \frac{\partial T}{\partial \vec{q}} = 0 \quad (3.20)$$

In a semi-classical approach, one would now expand S in powers of \hbar . In any case, the exact value of \hbar should not have physical significance, thus one would expect that the exact T and S are expandable in \hbar . It is then obvious from (3.19) that the the \hbar^0 -term of S should obey the same equation as W in (3.17), so

$$S = W + \mathcal{O}(\hbar) \quad (3.21)$$

Classical separability means that W can be written as a sum

$$W(\vec{q}) = W_1(q_1) + W_2(q_2) + \dots$$

Quantum-mechanical separability means that the wave-equation can be written as a product. Thus $\frac{i}{\hbar}S + T$ should be a sum, whose terms can be separated in a real and imaginary part, so both T and S should be a sum

$$\begin{aligned} S(\vec{q}) &= S_1(q_1) + S_2(q_2) + \dots \\ T(\vec{q}) &= T_1(q_1) + T_2(q_2) + \dots \end{aligned}$$

Now any of these terms can be expanded in powers of \hbar . From those expansions for the S_i , I could combine the \hbar^j -terms, and get a j -th order term that is a sum. So I see that in a separable quantum-mechanical systems, all terms are separable. But I already saw in (3.21), that the zero-th order term is exactly the classical W , which is therefore also a sum. Thus the classical version is separable. *Quantum-mechanical separability implies classical separability.* From this general statement, it is obvious that the quantum-mechanically separable systems in section 3.1.1 are also classically separable.

3.2.2 Stäckel Conditions

The fact that the systems found in section 3.1.1 are classically separable can also be view in a different way. There exist certain conditions in classical mechanics, called the *Stäckel conditions*; if these are fulfilled, the system is separable (Goldstein [11]). The condition are as follows:

If

- \mathcal{H} is conserved,
- \mathcal{H} is of the form $\mathcal{H} = \frac{1}{2}(\vec{p} - \vec{a})T(\vec{p} - \vec{a}) + V(\vec{q})$,
- The coordinates q_i form an orthogonal system, so T and T^{-1} are diagonal.

then the Hamilton-Jacobi equation is separable if

- \vec{a} has elements a_i that are functions only of the corresponding coordinate:
 $a_i = a_i(q_i)$,
- $V(\vec{q})$ can be written as a sum of the form

$$V(\vec{q}) = \sum_i \frac{V_i(q_i)}{T_{ii}}$$

- There exists a matrix Φ with elements $\Phi_{ij} = \Phi_{ij}(q_i)$ such that

$$(\Phi^{-1})_{1j} = \frac{1}{T_{jj}}$$

So then $W(\vec{q}) = \sum_i W_i(q_i)$ with W_i satisfying

$$\left[\frac{\partial W_i}{\partial q_i} - a_i \right]^2 = 2V_i(q_i) + 2\Phi_{ij}\gamma_j \quad (3.22)$$

where the γ_i are the constants of integration. Now I look at the systems of section 3.1.1, where all the conditions are seen to be satisfied, except the last one. Note that $T_{ii} = M$. I thus have to find a matrix Φ such that

$$\begin{pmatrix} M^{-1} & M^{-1} \\ A & B \end{pmatrix} \begin{pmatrix} \Phi_{11}(x_1) & \Phi_{12}(x_1) \\ \Phi_{21}(x_2) & \Phi_{22}(x_2) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

where A and B can be chosen freely.

$$\begin{pmatrix} M^{-1}[\Phi_{11}(x_1) + \Phi_{21}(x_2)] & M^{-1}[\Phi_{12}(x_1) + \Phi_{22}(x_2)] \\ A\Phi_{11}(x_1) + B\Phi_{21}(x_2) & A\Phi_{12}(x_1) + B\Phi_{22}(x_2) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Now M was a sum of two term, one a function of z and the other a function of θ , so I can choose Φ_{11} and Φ_{21} as these function to satisfy the (11) element of the equation. Since $M \neq 0$, the (12) element can only be satisfied if Φ_{12} and Φ_{22} are constant. I'll call $\Phi_{12} = \nu$, thus $\Phi_{22} = -\nu$. The (22) element is then satisfied when $A - B = \nu^{-1}$. Inserting this into the (21) element and solving B gives

$$B = -\frac{\Phi_{11}(x_1)}{M\nu}$$

So I can find A and B such that Φ exists and has the right properties. Therefore, all conditions are satisfied, and the systems are separable.

3.2.3 Construction of Classical Separable Billiards

Though I have now shown that all quantum-mechanically separable billiard are also separable classically, it remains to be seen if I have found all separable billiard. To see this, I can do an analogous construction as in section 3.1.1.

According to appendix C.3, the Hamiltonian in general coordinates looks like

$$\mathcal{H} = \frac{p_j (J^T J)_{jl} p_l}{2m} + V(q) \quad (3.23)$$

The Hamilton-Jacobi equation then becomes

$$\frac{\partial W}{\partial q_j} (J^T J)_{jl} \frac{\partial W}{\partial q_l} + V(q) = E \quad (3.24)$$

I try and separate $W = W_1(q_1) + W_2(q_2)$,

$$\sum_{j,l} \left\{ \frac{1}{2m} \frac{\partial W_j}{\partial q_j} (J^T J)_{jl} \frac{\partial W_l}{\partial q_l} \right\} + V(q) = E \quad (3.25)$$

When this is being separated, no multiplications with $\frac{\partial W_j}{\partial q_j}$ are required and therefore the general form of the separated equations is

$$A \left(\frac{\partial W_j}{\partial q_j} \right)^2 + V_j(q_j) = \sum_k \lambda_k f_k(q_j) \quad (3.26)$$

where $\lambda_1 = E$. A possible linear term $B \frac{\partial W_j}{\partial q_j}$ can be included in the quadratic term by a transformation $W \rightarrow W' = W + \frac{1}{2} \int \frac{A}{B} dq$. In two dimensions this becomes

$$\begin{aligned} \left(\frac{\partial W_1}{\partial q_1} \right)^2 + V_1(q_1) &= E f_1(q_1) + \lambda g_1(q_1) \\ \left(\frac{\partial W_2}{\partial q_2} \right)^2 + V_2(q_2) &= E f_2(q_2) + \lambda g_2(q_2) \end{aligned} \quad (3.27)$$

Eliminating λ and solving E gives

$$\frac{\partial W_j}{\partial q_j} A^{ji} \frac{\partial W_i}{\partial q_i} + \frac{g_2 V_1 - g_1 V_2}{f_1 g_2 - f_2 g_1} = E \quad (3.28)$$

where

$$A = \frac{1}{f_1 g_2 - f_2 g_1} \begin{pmatrix} g_2 & 0 \\ 0 & g_1 \end{pmatrix}$$

This expression has to be tied to the general expression (3.24), so $A = (J^T J)^{-1}$. Thus $J^T J$ is required to be diagonal, just as in section 3.1.1. One can therefore deduce that the kinetic energy term has to be of the form

$$\frac{1}{\det J} \left[\left(\frac{\partial W}{\partial q_1} \right)^2 + \left(\frac{\partial W}{\partial q_2} \right)^2 \right] \quad (3.29)$$

From $J^T J = 1$ it follows again that J is of the form (3.13). Analogous to the derivation in section 3.1.1, this means that the transformation is orthonormal.

From the separability condition, which is again that $M = \det J$ is a sum of part that depend on one coordinate only, I find the *same four types of separable systems* that I had quantum-mechanically.

Whittaker already derived in his famous book [24], of which the first edition was published in 1904, that "the only cases of motion of a particle in a plane under the action of conserved forces, which possesses an integral quadratic in the velocities other than the integral of energy, are those for which the potential energy has the form

$$V = \frac{f(\alpha) - \phi(\beta)}{\alpha^2 - \beta^2}$$

where α and β are the parameters of confocal ellipses and hyperbola". Indeed, the other three cases I found can be seen as degenerate cases of the ellipse, as illustrated in figure 34. Hietarinta found [14] eight integrable two-dimensional systems with a second constant of motion quadratic in the momenta. Eight of those however are complex: the other four can be shown to be the same are the four systems I found.

3.3 Examples

3.3.1 Parabolic Billiard

I will not treat the parabolic billiard as extensively as I did the elliptical billiard, but I would like to show some interesting similarities and differences between the two. This is considerably simplified by the results of section 3.1. Let me start by defining parabolic coordinates by $x + iy = \frac{1}{2}(z + i\theta)^2$ (so $f = \frac{1}{2}w^2$), explicitly

$$\begin{aligned} x &= \frac{1}{2}(z^2 - \theta^2) \\ y &= z\theta \end{aligned} \tag{3.30}$$

In these coordinates, the Hamiltonian becomes

$$\begin{aligned} \mathcal{H} &= \frac{-\hbar^2}{2m} \frac{1}{\left(\frac{\partial x}{\partial z}\right)^2 + \left(\frac{\partial x}{\partial \theta}\right)^2} \Delta_{z,\theta} \\ &= \frac{-\hbar^2}{2m} \frac{1}{z^2 + \theta^2} \Delta_{z,\theta} \end{aligned} \tag{3.31}$$

Lines of constant z are lying parabola that intersect the x -axis at $x = z^2/2$, and "point" leftwards. Similarly, lines of constant θ are parabola that intersect the x -axis at $x = -\theta^2/2$, and point rightwards. These parabola have the origin as their focal point. I take the lines $z = z_b$ and $\theta = \theta_b = z_b$ as the boundary of the billiard. The second conserved quantity is now

$$\mathcal{L}^2 = \frac{z^2 p_\theta^2 - \theta^2 p_z^2}{z^2 + \theta^2} \tag{3.32}$$

This quantity can actually also be interpreted as the product of the angular momenta with respect to the focal points, but now the second focal point is at $(-F, 0)$ with $F \rightarrow \infty$. Therefore

$$\frac{l_2}{F} = \frac{(x+F)p_y - yp_x}{F} \rightarrow p_y \quad (3.33)$$

and since $l_1 = l_z$, the second constant of motion reduces to $l_z p_y$ or, symmetrized,

$$\mathcal{L}^2 = \frac{1}{2}(l_z p_y + p_y l_z) \quad (3.34)$$

Notice that it doesn't matter whether F is negative or positive, and therefore \mathcal{L}^2 is conserved in collisions both with the left wall and the right wall. The separated problem becomes

$$\begin{aligned} -\frac{\hbar^2}{2m}\partial_z^2 Y + \lambda Y + E z^2 Y &= 0 \\ -\frac{\hbar^2}{2m}\partial_\theta^2 T - \lambda T + E \theta^2 T &= 0 \end{aligned} \quad (3.35)$$

which can be interpreted as an eigenvalue problem for \mathcal{L}^2 as well as for \mathcal{H} . Notice that inserting $z \rightarrow i\theta$ in the first equation gives the second, so the problem can also be formulated in the complex plane. The equations also show that under $z \leftrightarrow \theta$ all that happens is that λ changes sign. E is unchanged, and since the transformation is just a reflection in the y -axis, which leaves the billiard unchanged, this means that I have a degeneracy: for each state $|E; \lambda\rangle$ there exists a state $|E; -\lambda\rangle$. This is due to the mirror symmetry in the y -axis, which in the case of the ellipse could be removed by looking at one quadrant, and the symmetry did not introduce any degeneracies. Here there is no line $z = z_0$ or $\theta = \theta_0$ that coincides with the y -axis, so this cannot be done without destroying the separability. However, once I have the states $|E; \lambda\rangle$ and $|E; -\lambda\rangle$, I can easily construct eigenstate of \mathcal{H} that are also eigenstates of π_y , namely $\frac{1}{\sqrt{2}}(|E; \lambda\rangle + |E; -\lambda\rangle)$ and $\frac{1}{\sqrt{2}}(|E; \lambda\rangle - |E; -\lambda\rangle)$, since $\pi_y |E; \lambda\rangle = |E; -\lambda\rangle$. More general parabolic billiards can be constructed that do not have mirror symmetry in the y -axis, by choosing $z_b \neq \theta_b$, and those do not have the degeneracy.

In general, to make \mathcal{L}^2 really conserved, I have to add

$$X = \frac{\theta^2 V_1 - z^2 V_2}{\theta^2 + z^2} \quad (3.36)$$

to \mathcal{L}^2 , and \mathcal{H} has to have a potential of the form

$$V = \frac{V_1(z) + V_2(\theta)}{\theta^2 + z^2} \quad (3.37)$$

Unfortunately, none of the parabolic coordinates is periodic, so the asymptotic method I used in section 2.2 cannot be used. Also, I have not been able to find I nice deformation to a geometric shape of which the eigenfunctions are known and for which matrix elements are easily computed, like Ayant and Arvieu[1] had for the ellipse.

3.3.2 Circular Billiard

Though this example is well-studied, it is illuminating to review it in the light of the theory developed above. This will also show why this example (as well as the one in the next section) is not so problematic as the elliptical and the parabolical billiards. Let me define circular coordinates slightly different than they are conventionally defined, by $x + iy = e^{z+i\theta}$ (so $f = e^w$), or explicitly

$$\begin{aligned}x &= e^z \cos \theta \\y &= e^z \sin \theta\end{aligned}\tag{3.38}$$

In these coordinates, the Hamiltonian becomes

$$\begin{aligned}\mathcal{H} &= \frac{-\hbar^2}{2m} \frac{1}{\left(\frac{\partial x}{\partial z}\right)^2 + \left(\frac{\partial x}{\partial \theta}\right)^2} \Delta_{z,\theta} \\ &= \frac{-\hbar^2}{2m} \frac{1}{e^{2z}} \Delta_{z,\theta}\end{aligned}\tag{3.39}$$

Lines of constant z are of course circles with radius e^z , lines of constant θ are straight lines from the origin at an angle θ with respect to the positive x -axis. A line $z = z_b$ is taken to be the boundary of the billiard. The second conserved quantity is now

$$\mathcal{L}^2 = p_\theta^2\tag{3.40}$$

Since this quantity is the square of l_z , this means that l_z is conserved. Note that again this quantity is the product of the angular momenta with respect to two focal points, but now these focal points coincide at the origin. The separated problem becomes

$$-\frac{\hbar^2}{2m} \partial_z^2 Y + \lambda Y + E e^{2z} Y = 0\tag{3.41}$$

$$-\frac{\hbar^2}{2m} \partial_\theta^2 T - \lambda T = 0\tag{3.42}$$

which cannot be interpreted as an eigenvalue problem for \mathcal{L}^2 as well as for \mathcal{H} : the last equation is the full eigenvalue problem of \mathcal{L}^2 . No formulation in the complex plane exists. Notice that to make \mathcal{L}^2 really conserved, I need to add

$$X = -V_2(\theta)\tag{3.43}$$

to \mathcal{L}^2 , when \mathcal{H} then has to have a potential of the form

$$\begin{aligned}V &= \frac{V_1(z) + V_2(\theta)}{e^{2z}} \\ &= \frac{V_2(\theta)}{r^2} + \tilde{V}(r)\end{aligned}\tag{3.44}$$

where r is the conventional radial coordinate. A special case of this is $V_2 \equiv 0$, which means I have a circular symmetric potential, in which case I know that l_z is conserved. It is the fact that (3.42) is enough to determine the eigenvalues and functions of \mathcal{L}^2 , that allows one to first solve the problem for l_z , and then use that to find solutions to (3.41). In the other cases I have considered neither of the two separated equations could be solved independently.

3.3.3 Rectangular Billiard

This last example is the simplest of all separable billiards. No new coordinates are required, and $\mathcal{H} = \frac{1}{2m}\Delta$. The conserved quantity in this case is

$$\mathcal{L}^2 = p_y^2 \quad (3.45)$$

Which is again $l_1 l_2$ with $l_1 \rightarrow -Fp_y$ and $l_2 \rightarrow Fp_y$. The separated problem is now

$$\partial_x^2 X = (-E + \lambda)X \quad (3.46)$$

$$\partial_y^2 Y = -\lambda Y \quad (3.47)$$

giving $E \sim n^2 + \alpha m^2$, if α is the square of the ratio of the sides. One should actually add a term $X = V_2(\theta) - V_1(z)$ to \mathcal{L}^2 , where V should be of the form $V = V_1(z) + V_2(\theta)$, to make this a separable problem. Again (3.47) can be solved independently of (3.46), which makes separation a fruitful approach in this case.

4 Conclusion

This thesis was about the borderline between chaos and regular behavior in quantum mechanics. I looked at a class of two-dimensional systems that are separable classically and, formally, also quantum-mechanically. Because the equations I get by separating, both contain the separation constant and the eigenvalue, they are not really separable. Specifically, I looked at an elliptical billiard. In literature, level repulsion under variation of a parameter is called one of the characteristics of quantum-chaotic systems. The arguments that regular systems do not exhibit repulsion generically, seem to be based on solved examples, so they do not need to have absolute validity. To say anything about the generic behavior of energy-levels, I needed a large number of eigenvalues. Calculating those proved to be a difficult task. Direct solvation was impossible. Numerically, methods proved to be either too time-consuming (direct diagonalization) or too inaccurate (Lanczos method). Nor was I able to show that degeneracies do not occur at all.

I did manage to find an asymptotic approximation, that is senseless to zeroth order – the statistical quantities can become undefined [5] – but starts to make sense when higher correction terms are included. In this approximation, the levels crossed. Also the statistical quantities of the eigenvalues $P(s)$ and $\bar{\Delta}_3(L)$, that indicate whether a spectrum is chaotic look like those of a regular spectrum.

A numerical calculation of just a few dozen of the lowest eigenvalues show crossing of levels. This is in contradiction with similar calculations performed by Ayant and Arvieu [1], who show in their figures a clear repulsion of some of the levels, which I do not find. I suspect that they used a diagonalization routine that is unstable for degenerated states. Numerical errors can generically cause seemingly undegenerate states, but not create degenerate states. Above that, there is also analytic evidence of crossing, as is discussed in section 2.2.8.

Finally, the elliptical billiard can be seen as the *Mother of all Real Separable Billiards* in two dimensions, in the sense that all four types of separable billiard found in the last part can be seen as degenerations of a billiard of which the boundaries are lines of constant z or θ , in elliptic coordinates. This is illustrated in figure 34. The parabolic billiard will show the same kind of problems as the elliptical billiard, while the rectangular and circular billiard will not.

Despite of the problems, I thus arrived at some results after all on this easily defined problem, which seemed to get less accessible with every new approach. That I didn't find any "Quantum Chaos", that's just the way it is.

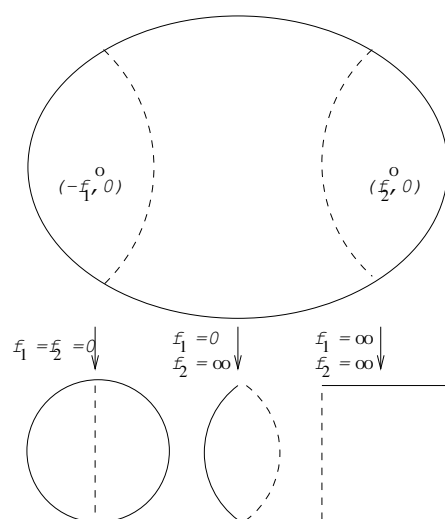


Figure 34: The Mother of Separable Billiards.

Appendices

In these appendices I'll discuss first some classical concepts, then I will treat some concepts related to Quantum Chaos. After that, some technicalities follow, the last of which are specific for the problems discussed in the previous sections. Finally, the numerical methods I used are described briefly.

A Aspects of the Classical Formalism

A.1 The Lagrangian vs. the Hamiltonian

When one performs a change of position-coordinates, it is not immediately clear how the Hamiltonian should change. It is then easier to use the Lagrangian, in the following way.

When the Hamiltonian $\mathcal{H} = T + V$ does not depend on time explicitly, the *Lagrangian* becomes $L = T - V$, which is to be considered a function of x , y , \dot{x} and \dot{y} . The equations of motion can be found from the *Euler-Lagrange equations*

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) = 0$$

The *generalized momenta* are defined as

$$\begin{aligned} p_x &= \frac{\partial L}{\partial \dot{x}} \\ p_y &= \frac{\partial L}{\partial \dot{y}} \end{aligned} \quad (\text{A.1})$$

Then the Hamiltonian can be retrieved by its definition in the Lagrangian formalism:

$$\mathcal{H} = \dot{x}(x, y, p_x, p_y)p_x + \dot{y}(x, y, p_x, p_y)p_y - L(x, y, p_x, p_y) \quad (\text{A.2})$$

which is considered a function of x , y , p_x and p_y . The equations of motion are found from *Hamilton's equations*:

$$\begin{aligned} \dot{x} &= \frac{\partial \mathcal{H}}{\partial p_x} \quad , \quad \dot{p}_x = -\frac{\partial \mathcal{H}}{\partial x} \\ \dot{y} &= \frac{\partial \mathcal{H}}{\partial p_y} \quad , \quad \dot{p}_y = -\frac{\partial \mathcal{H}}{\partial y} \end{aligned} \quad (\text{A.3})$$

These will coincide with the equations of motion found from the Euler-Lagrange equations.

The *Poisson-brackets* are defined, as usually, by

$$\{A, B\} = \frac{\partial A}{\partial \vec{q}} \cdot \frac{\partial B}{\partial \vec{p}} - \frac{\partial A}{\partial \vec{p}} \cdot \frac{\partial B}{\partial \vec{q}} \quad (\text{A.4})$$

Using Hamilton's equations, the time evolution of a quantity $A(\vec{p}, \vec{q}, t)$, is given by

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \{A, \mathcal{H}\} \quad (\text{A.5})$$

A quantity is clearly conserved, if the Poisson-bracket with the Hamiltonian is zero.

A.2 Canonical Transformations and the Hamilton-Jacobi Equation

In this section, I will explain the Hamilton-Jacobi formalism. *Canonical transformations* are coordinate-momenta transformations

$$\begin{aligned} (\vec{p}, \vec{q}) &\rightarrow (\vec{P}, \vec{Q}) \\ P_i = P_i(\vec{p}, \vec{q}, t) &\text{ and } Q_i = Q_i(\vec{p}, \vec{q}, t) \end{aligned} \quad (\text{A.6})$$

that preserve the *Poisson-brackets* relations between coordinates and momenta:

$$\begin{aligned} \{Q_k, Q_l\} &= 0 \\ \{P_k, P_l\} &= 0 \\ \{Q_k, P_l\} &= \delta_{kl} \end{aligned} \quad (\text{A.7})$$

Under this condition Hamilton's equations of motion remain the same. It can be shown that these transformation are determined by a *generating function* S as follows: let S be some function of \vec{q} , \vec{Q} and t . The *generalized momenta* as can be found by

$$\vec{p} = \frac{\partial S}{\partial \vec{q}} \quad (\text{A.8})$$

$$\vec{P} = -\frac{\partial S}{\partial \vec{Q}} \quad (\text{A.9})$$

while the new Hamiltonian is

$$\mathcal{H}' = \mathcal{H}(\vec{p}, \vec{q}, t) + \frac{\partial S}{\partial t}(\vec{q}, \vec{Q}, t) \quad (\text{A.10})$$

At this point the expressions are in terms of \vec{q} , \vec{Q} . To find them in terms of \vec{q} and \vec{p} , \vec{Q} should be extracted from (A.8) and then inserted into (A.9) and (A.10). Note that if the Hamiltonian doesn't depend explicitly on time it is unchanged except for the change in variables. The transformation $(\vec{p}, \vec{q}) \rightarrow (\vec{P}, \vec{Q})$ is canonical. As one sees the Hamiltonian can be transformed into a different form by a canonical transformation. This new form may give simpler Hamilton's equations. A particular simple form of the new Hamiltonian would be $\mathcal{H}' = 0$. In that case Hamilton's equation of motion would state that the coordinates and momenta \vec{Q} and \vec{P} are constant. If one knows the expressions for the transformation $\vec{p}(\vec{P}, \vec{Q}, t)$, $\vec{q}(\vec{P}, \vec{Q}, t)$ and the inverses $\vec{P}(\vec{p}, \vec{q}, t)$, $\vec{Q}(\vec{p}, \vec{q}, t)$, the solution to the problem with initial values $\vec{p}(0) = \vec{p}_0$, $\vec{q}(0) = \vec{q}_0$ is given by $\vec{q}(t) = \vec{q}[\vec{P}(\vec{p}_0, \vec{q}_0, 0), \vec{Q}(\vec{p}_0, \vec{q}_0, 0), t]$ and $\vec{p}(t) = \vec{p}[\vec{P}(\vec{p}_0, \vec{q}_0, 0), \vec{Q}(\vec{p}_0, \vec{q}_0, 0), t]$. This possibility does not help if finding such a canonical transformation is very difficult. Remembering, however, that a canonical transformation is given by a generating function $S(\vec{q}, \vec{Q}, t)$, one sees from (A.10) that H' becomes zero if

$$\frac{\partial S(\vec{q}, t)}{\partial t} + \mathcal{H}\left(\frac{\partial S(\vec{q}, t)}{\partial \vec{q}}, \vec{q}, t\right) = 0 \quad (\text{A.11})$$

in which I dropped the \vec{Q} dependence. This equation is called the Hamilton-Jacobi equation. If a solution which has n constants of integration (where n is the dimension of the \vec{q} and \vec{p} vectors) can be found, it is called a complete solution. Equation (A.11) does not state anything on the dependence of S on \vec{Q} explicitly, so the constants of integration can be used to define the new generalized coordinates \vec{Q} . The solution of the problem has by now boiled down to the solution of a partial differential equation for a scalar function S . A slightly alternative approach is possible by performing a so-called Legendre transformation $S \rightarrow S' = S + Q_l P_l$, thus looking for a generating function $S(\vec{q}, \vec{P}, t)$, which again satisfies (A.11). The constants of integration now define \vec{P} . Then \vec{q} should be extracted from

$$\vec{Q} = \frac{\partial S}{\partial \vec{P}} \quad (\text{A.12})$$

Then the momenta \vec{p} are to be found using (A.8). The constants of integration can be seen as constants of the motion, since they do not change in time. One easily sees that for a time-independent Hamiltonian: write

$$S = W - Et \quad (\text{A.13})$$

Substitution in (A.11) then gives

$$\mathcal{H}\left(\frac{\partial W}{\partial \vec{q}}, \vec{q}\right) = E \quad (\text{A.14})$$

Thus I have separated the time-variable gaining a constant of integration E , which thus is a constant of the motion. Equation (A.14) can be seen as a time-independent Hamilton-Jacobi equation. In many cases such a separation can be pursued further. The general strategy of separation for the Hamilton-Jacobi equation is to write

$$W(\vec{Q}) = W_1(Q_1) + W_r(Q_2, \dots, Q_n) \quad (\text{A.15})$$

Substitute this into (A.14) and hope that the resulting equation can be written as $A = B$, with A dependent only on Q_1 and B not dependent on Q_1 . Then both A and B should be equal to some constant λ and the equation separates into $A = \lambda$ and $B = \lambda$. This may be continued until equations containing only one variable are left, which are n ordinary differential equations. If this can be done the system is said to be separable. Having all the constants of the motion, the problem would be solved if the n equations in terms of the constants of the motion could be solved.

B Aspects of Quantum Chaos vs. Regularity

B.1 Commutators and Time Evolution

In quantum mechanics, the *commutator* of two quantities A and B is

$$[A, B] = AB - BA \quad (\text{B.1})$$

Dirac showed in [10] that this can be viewed as the analogue of Poisson-brackets, in the sense that it has the same properties but its arguments are non-commuting objects. A general rule is suggested that the value of commutator of two quantities in terms of p and q is $i\hbar$ times the value of the Poissonbrackets of their classical counterparts. The assignment of such counterparts is however not unique – one has to take some ordering convention – nor can this rule be proved. In a mathematical jargon, Poisson brackets and commutators have a different algebra.

Turning again to time evolution, The (formal) solution of the time dependent Schrödinger equation is

$$\Psi(t) = U_{t-t_0}\Psi(t_0) \quad (\text{B.2})$$

where

$$U_{t-t_0} = \exp[-i\mathcal{H}(t-t_0)/\hbar]$$

Using the definition of the *expectation value*

$$\langle A \rangle = \langle \Psi(t) | A | \Psi(t) \rangle$$

one can find

$$\frac{d}{dt}\langle A \rangle = \left\langle \frac{\partial A}{\partial t} + \frac{1}{i\hbar}[A, \mathcal{H}] \right\rangle \quad (\text{B.3})$$

which is rather analogous to (A.5).

As in classical mechanics, a quantity $A(p, q)$ is conserved ($\frac{dA}{dt} = 0$) if the commutator with the Hamiltonian is zero. These two analogies confirm the general rule.

B.2 Two-by-two Matrix Approximation for Approaching levels

In this section the approximation by a two-by-two matrix will be justified. I will do this by means of an explicit construction of that matrix. When looking for eigenvalues of \mathcal{H} , one has to solve

$$\begin{aligned} \det(\mathcal{H} - EI) &= \prod_i (E - E_i) \\ &= (E - E_1)(E - E_2) \prod_{i>2} (E - E_i) \\ &= 0 \end{aligned} \quad (\text{B.4})$$

Now I'm interested in two neighbouring levels as a function of the parameter ϵ . Denote these two levels by E_1 and E_2 . Suppose all eigenfunctions are known at $\epsilon = 0$. They form the basis $\{|1\rangle, |2\rangle, |3\rangle, \dots\}$. Suppose for the moment that the eigenfunctions corresponding to the levels E_3, E_4, \dots are known for all ϵ , and call them $|\phi_{j>2}^{(\epsilon)}\rangle$. I now define the operator

$$P^{(\epsilon)} = \sum_{j>2} |\phi_j^{(\epsilon)}\rangle \langle \phi_j^{(\epsilon)}| \quad (\text{B.5})$$

For any ϵ , I can complete the basis $|\phi_{j>2}^{(\epsilon)}\rangle$ by

$$\begin{aligned} |\phi_1^{(\epsilon)}\rangle &= |1\rangle - P^{(\epsilon)}|1\rangle \\ |\phi_2^{(\epsilon)}\rangle &= |2\rangle - P^{(\epsilon)}|1\rangle \end{aligned} \quad (\text{B.6})$$

This basis is not orthonormal, since for $i, j < 3$

$$\langle \phi_i^{(\epsilon)} | \phi_j^{(\epsilon)} \rangle = \delta_{ij} - \langle i | P^{(\epsilon)} | j \rangle \quad (\text{B.7})$$

On this basis, \mathcal{H} takes on the – block-diagonal – form

$$\mathcal{H}^{(\epsilon)} = \begin{pmatrix} A_{ij}^{(\epsilon)} & & & \\ & E_3 & & \\ & & E_4 & \\ & & & \ddots \end{pmatrix} \quad (\text{B.8})$$

with

$$A_{ij}^{(\epsilon)} = \langle \phi_i^{(\epsilon)} | \mathcal{H}^{(\epsilon)} | \phi_j^{(\epsilon)} \rangle$$

for $i, j < 3$. I can write

$$\begin{aligned} A_{ij}^{(\epsilon)} &= \langle i | \mathcal{H}^{(\epsilon)} | j \rangle \\ &+ \langle i | -P^{(\epsilon)}\mathcal{H}^{(\epsilon)} - \mathcal{H}^{(\epsilon)}P^{(\epsilon)} + P^{(\epsilon)}\mathcal{H}^{(\epsilon)}P^{(\epsilon)} | j \rangle \end{aligned} \quad (\text{B.9})$$

Since $[\mathcal{H}, P] = 0$ and $P^2 = P$ for all ϵ ,

$$-P^{(\epsilon)}\mathcal{H}^{(\epsilon)} - \mathcal{H}^{(\epsilon)}P^{(\epsilon)} + P^{(\epsilon)}\mathcal{H}^{(\epsilon)}P^{(\epsilon)} = -P^{(\epsilon)}\mathcal{H}^{(\epsilon)}$$

so

$$A_{ij}^{(\epsilon)} = \langle i | \mathcal{H}^{(\epsilon)} | j \rangle - \sum_{l>2} E_l \langle i | \phi_l^{(\epsilon)} \rangle \langle \phi_l^{(\epsilon)} | j \rangle \quad (\text{B.10})$$

Now I look at this from a perturbative point of view, and assume that

$$|\phi_{l>2}^{(\epsilon)}\rangle = |l\rangle + \epsilon |\Psi_l\rangle + \mathcal{O}(\epsilon^2) \quad (\text{B.11})$$

Substituting this into (B.7) and (B.10), I get

$$\begin{aligned} \langle \phi_i^{(\epsilon)} | \phi_j^{(\epsilon)} \rangle &= \delta_{ij} + \mathcal{O}(\epsilon^2) \\ A_{ij}^{(\epsilon)} &= \langle i | \mathcal{H}^{(\epsilon)} | j \rangle \mathcal{O}(\epsilon^2) \end{aligned} \quad (\text{B.12})$$

So I see that to first order in ϵ , \mathcal{H} can be modeled by a two-by-two matrix formed by matrix elements of \mathcal{H} on the fixed basis $\{|j\rangle\}$. This also means that if random matrix theory can be applied to the whole \mathcal{H} , it can also be applied on $A_{ij}^{(\epsilon)}$ with the same measure on the matrix elements, since no randomness is in the basis up to $\mathcal{O}(\epsilon)$. Note that at this point there is no more need for the assumption that the $|\phi_{j>2}^{(\epsilon)}\rangle$ are known. There's an argument why for near

degenerate levels the approximation is also very good up to $\mathcal{O}(\epsilon^2)$. It follows from the standard result in perturbation theory for the eigenvalues $E_i^{(\epsilon)}$ of a Hamiltonian $\mathcal{H}_0 + \epsilon\mathcal{H}_1$:

$$E_i^{(\epsilon)} = E_i + \epsilon \langle i | \mathcal{H}_1 | i \rangle + \epsilon^2 \sum_{i \neq j} \frac{|\langle i | \mathcal{H}_1 | j \rangle|^2}{E_i - E_j} + \mathcal{O}(\epsilon^3) \quad (\text{B.13})$$

So I see that the behavior of E_i is dominated by the levels which are close to it, since then $\frac{1}{E_i - E_j}$ becomes large. This indicates that a two-by-two matrix is a good approximation for the behavior of those two approaching energy levels.

B.3 Derivation of $P(H)$ and $P(E_+, E_-)$

In this section the formulae (2.10) and (2.11) are derived, using Random Matrix Theory[13, 17]. I will only consider the *Gaussian ensemble of hermitian matrices*, also called *GUE*, which are of the form (2.5). Besides having to be normalized to unity, there are two other requirements:

- The density should be insensitive to a change of base, so

$$P(H) = P(U^\dagger H U) \quad (\text{B.14})$$

where U is a unitary matrix.

- The distribution should be such that H_{11} , H_{22} and H_{12} are independent, so

$$P(H) = P_{11}(H_{11})P_{22}(H_{22})P_{12}(H_{12}, H_{12}^*) \quad (\text{B.15})$$

All invariants of H under a unitary transformation can be expressed in traces over powers of H . In two dimensions, there are two invariants, so

$$t_1 = \text{Tr } H \quad t_2 = \text{Tr } H^2$$

suffice and $P(H)$ is a function of those according to the first requirement. Now note that

$$t_1 = H_{11} + H_{22} \quad t_2 = H_{11}^2 + H_{22}^2 + 2 |H_{12}|^2 \quad (\text{B.16})$$

so P_{12} should be a function of $|H_{12}|^2$ only. Defining

$$\begin{aligned} W &= \ln P \\ W_{11} &= \ln P_{11} \\ W_{22} &= \ln P_{22} \\ W_{12} &= \ln P_{12} \end{aligned}$$

the last requirement takes on the form

$$W(t_2, t_1) = W_{11}(H_{11}) + W_{22}(H_{22}) + W_{12}(|H_{12}|^2)$$

Differentiating this with respect to H_{11} , H_{22} and $|H_{12}|^2$, using (B.16), gives me

$$\frac{\partial W}{\partial t_2} = \frac{1}{2}W'_{12} \quad (\text{B.17})$$

$$\frac{\partial W}{\partial t_1} = W'_{11} - W'_{12}H_{11} \quad (\text{B.18})$$

$$\frac{\partial W}{\partial t_1} = W'_{22} - W'_{12}H_{22} \quad (\text{B.19})$$

where primes denote differentiation to their (exclusive) argument and I already used (B.17) to get (B.18) and (B.19). Equating these last two gives

$$\frac{W'_{11} - W'_{22}}{H_{11} - H_{22}} = W'_{12}$$

Since the left hand side contains terms in H_{11} and H_{22} and the right hand side contains terms in $|H_{12}|^2$ only, I see that W'_{12} has to be a constant, which I define as $-2A$. Inserting this into the last equation then gives me

$$W'_{11} + 2AH_{11} = W'_{22} + 2AH_{22}$$

of which both sides should equal the same constant ν again. Inserting that into (B.18) and (B.19) leads to the same expressions:

$$\frac{\partial W}{\partial t_1} = \nu$$

Together with (B.17),

$$\frac{\partial W}{\partial t_2} = -A \quad (\text{B.20})$$

one easily obtains the general formula for $P(H) = \exp(W(t_2, t_1))$:

$$P(H) = C \exp(-A \text{Tr } H^2 + \nu \text{Tr } H)$$

The minus sign in front of A was put there to make this normalizable – since H will be bounded from below, but not from above. In the subsequent discussion any C in front of a density is to be understood as a constant to be determined by normalization. I can get rid of the linear term by a shift in the zero of energy by an amount of $\frac{\nu}{A}$, thus

$$P(H) = C \exp(-A \text{Tr } H^2) \quad (\text{B.21})$$

which is exactly (2.10). This distribution is in terms of H_{11}, H_{22}, H_{12} and H_{12}^* . Any hermitian two by two matrix can be written as a transformed diagonal matrix $H = U^\dagger \text{diag}(E_+, E_-)U$, where U a unitary matrix

$$U = \begin{pmatrix} \cos \theta & e^{i\phi} \sin \theta \\ -e^{-i\phi} \sin \theta & \cos \theta \end{pmatrix}$$

So I can perform a transformation of variables to E_+ , E_- , θ and ϕ . The distribution then needs to be multiplied by the Jacobian

$$\begin{aligned} J &= \det \frac{\partial(H_{11}, H_{22}, H_{12}, H_{12}^*)}{\partial(E_+, E_-, \theta, \phi)} \\ &= g(\theta, \phi)(E_+ - E_-)^2 \end{aligned}$$

The explicit form of the function $g(\theta, \phi)$ is not needed when I perform a partial integration with respect to ϕ and θ of $P(H)$, since it only gives some factor which can be obtained by the normalization-requirement too. This gives me the distribution of eigenvalues of H , which thus becomes

$$P(E_+, E_-) = C(E_+ - E_-)^2 e^{-A(E_+^2 + E_-^2)} \quad (\text{B.22})$$

which is again (2.11).

B.4 Expressions for $P(s)$

From equation (B.22), the level spacing distribution can easily be obtained, since by definition

$$P(s) = \int dE_+ \int dE_- \delta(s - |E_+ - E_-|) P(E_+, E_-) \quad (\text{B.23})$$

so for the GUE

$$P(s) = C \int dE_+ \int dE_- \delta(s - |E_+ - E_-|) (E_+ - E_-)^2 e^{-A(E_+^2 + E_-^2)}$$

Via a change of variables to $E = E_+ + E_-$ and $s' = E_+ - E_-$, all the s -dependent terms factorize, so that the E -integral can be done and put into the normalization constant, leaving

$$P(s) = C \int ds' \delta(s - s') s'^2 e^{-2As'^2}$$

which is trivially solved. After setting the mean spacing to unity

$$1 = \int ds s P(s)$$

and determining C , I find

$$P(s) = \frac{32}{\pi^2} s^2 e^{-\frac{4}{\pi}s^2} \quad (\text{B.24})$$

One could have taken other ensembles, which require invariance of $P(H)$ under *orthogonal* (GOE) or *symplectic* transformations (GSE). These give analogous results:

$$P(s) = \begin{cases} \frac{\pi}{2} s e^{-\frac{\pi}{4}s^2} & \text{orthogonal} \\ \frac{2^{18}}{3^6 \pi^3} s^4 e^{-\frac{64}{9\pi}s^2} & \text{symplectic} \end{cases} \quad (\text{B.25})$$

From $P(0) = 0$, one sees that these spectra show level repulsion. For regular spectra the random matrix approach does not work, since the allowed transformations depend on the character of the constants of motion. From (2.8) I could suspect that the energies in such a system are totally independent. If the energy-spectrum is scaled such that an energy-level is equally probable at all scales (the energies are Poissonian distributed), the following derivation can be done[17]. I want to know the probability that given an energy level at E , the next energy level is between $E + s$ and $E + s + ds$, which is $P(s)ds$. To determine this, I divide the interval from E to $E + s$ in M parts. Since I assume that the energy levels are totally uncorrelated, the chance of finding an energy level in such a part is the same for all parts. If I normalize the density of states to be 1, then this chance is $\frac{s}{M}$. Then $P(s)ds$ is given by the product of the probabilities that the next level is not in any of the parts, multiplied by the probability that it lies between $E + s$ and $E + s + ds$, which is just ds , thus

$$\begin{aligned} P(s)ds &= \lim_{M \rightarrow \infty} \prod_{i=0}^{M-1} \left(1 - \frac{s}{M}\right) ds \\ &= \lim_{M \rightarrow \infty} \left[1 - \frac{s}{M}\right]^M ds \end{aligned} \quad (\text{B.26})$$

taking this limit, I get

$$P(s) = e^{-s} \quad (\text{B.27})$$

Therefore this distribution for level spacings is the expected distribution for regular spectra, which is often called the *Poisson distribution* in this context. For the random-matrix distributions this approach does not work because one doesn't have an explicit expression for the probability that a level is between $E + s$ and $E + s + ds$, given that there is a level at E . If I knew that probability, let me call it $g(s)ds$, it is not difficult to redo the above construction, and I get

$$P(s)ds = \lim_{M \rightarrow \infty} \prod_{i=0}^{M-1} \left[1 - \frac{s}{M} g\left(i \frac{s}{M}\right)\right] g(s)ds \quad (\text{B.28})$$

Using

$$\prod_i (1 - f(i) dx) \approx \exp \left[- \sum_i f(i) dx \right] \quad (dx \text{ small})$$

the sum becomes an integral in (B.28), so it becomes

$$P(s) = g(s) \exp \left[- \int_0^s ds' g(s') \right] \quad (\text{B.29})$$

For uncorrelated levels, $g(s) = 1$, I regain (2.13). From the last expression, I can also derive that

$$g(s) = \frac{P(s)}{1 - \int_0^s ds' P(s')} \quad (\text{B.30})$$

so for the random-matrix distributions, the $g(s)$ becomes a complicated function of s , which cannot be known a priori.

B.5 Expressions for $\bar{\Delta}_3(L)$

The *spectral rigidity* $\bar{\Delta}_3$ is defined by

$$\begin{aligned}\bar{\Delta}_3(L) &= \left\langle \min_{a,b} \frac{1}{L} \int_{E-\frac{L}{2}}^{E+\frac{L}{2}} (N(E') - a - bE')^2 dE' \right\rangle \\ &= \left\langle \sigma\left(E - \frac{L}{2}, L\right) \right\rangle\end{aligned}\quad (\text{B.31})$$

where $\langle \rangle$ denotes an average over E , and σ is

$$\sigma(E, L) = \min_{a,b} \frac{1}{L} \int_E^{E+L} (N(E') - a - bE')^2 dE' \quad (\text{B.32})$$

The shift over $\frac{L}{2}$ is of no influence because of the averaging. Using the properties of the minimum, one easily finds

$$\begin{aligned}\sigma(E, L_1 + L_2) &\geq \frac{1}{L_1 + L_2} \left[\min_{a,b} \int_E^{E+L_1} (N(E') - a - bE')^2 dE' + \min_{a,b} \int_{E+L_1}^{E+L_1+L_2} (N(E') - a - bE')^2 dE' \right] \\ &= \frac{L_1}{L_1 + L_2} \sigma(E, L_1) + \frac{L_2}{L_1 + L_2} \sigma(E + L_1, L_2)\end{aligned}$$

taking the average over E , this becomes

$$(L_1 + L_2) \bar{\Delta}_3(L_1 + L_2) \geq L_1 \bar{\Delta}_3(L_1) + L_2 \bar{\Delta}_3(L_2) \quad (\text{B.33})$$

Now look at

$$\begin{aligned}\frac{d}{dL} [L \bar{\Delta}_3(L)] &= \lim_{dL \rightarrow 0} \frac{(L + dL) \bar{\Delta}_3(L + dL) - L \bar{\Delta}_3(L)}{dL} \\ &\geq \lim_{dL \rightarrow 0} \frac{L \bar{\Delta}_3(L) + dL \bar{\Delta}_3(dL) - L \bar{\Delta}_3(L)}{dL} \\ &= \bar{\Delta}_3(0)\end{aligned}$$

Now $\bar{\Delta}_3 \geq 0$, so this means that $L \bar{\Delta}_3(L)$ is an increasing function.

If I take $L_1 = L_2 = L$ in (B.33), I find

$$\bar{\Delta}_3(2L) \geq \bar{\Delta}_3(L)$$

I can also give estimates of $\bar{\Delta}_3(nL)$, using (B.33) until only terms in $\bar{\Delta}_3(L)$ remain. This gives

$$\bar{\Delta}_3(nL) \geq \bar{\Delta}_3(L) \quad (\text{B.34})$$

so $\bar{\Delta}_3(L)$ is in a sense a globally increasing function.

It is useful to write σ explicitly in terms of the spectrum, using

$$N(E) = \sum_i \Theta(E - E_i)$$

which can be integrated explicitly. In this way I find

$$\sigma(E, L) = J(E, L) - [R(E, L)]^2 - 3[C(E, L)]^2 \quad (\text{B.35})$$

where

$$\begin{aligned}
 J(E, L) &= \sum_{i=i_{min}}^{i_{max}} (2(i - i_{min}) + 1) \left(1 - \frac{E_i - E_0}{L}\right) \\
 R(E, L) &= \sum_{i=i_{min}}^{i_{max}} \left(1 - \frac{E_i - E_0}{L}\right) \\
 C(E, L) &= \sum_{i=i_{min}}^{i_{max}} \frac{E_i - E_0}{L} \left(1 - \frac{E_i - E_0}{L}\right)
 \end{aligned} \tag{B.36}$$

i_{min} and i_{max} are such that all energy-levels between E and $E + L$ are included. The expression for $\bar{\Delta}_3$ becomes

$$\bar{\Delta}_3(L) = \langle J(E, L) \rangle - \langle [R(E, L)]^2 \rangle - 3 \langle [C(E, L)]^2 \rangle \tag{B.37}$$

Using these expressions, I can calculate $\bar{\Delta}_3$ for some cases. First I look at small L . For an unfolded spectrum, the average level spacing is 1, so for $L < 1$, it suffices to look at one energy level to calculate σ . The interval $[E, E + L]$ is totally flat for a fraction of $\frac{1-L}{1}$ of the values of E , in which case $\sigma = 0$. For other E -values, one energy level is in the interval, let's say at $E + x_s$ so

$$\begin{aligned}
 J &= \left(1 - \frac{x_s}{L}\right) \\
 R &= \left(1 - \frac{x_s}{L}\right) \\
 R &= \left(1 - \frac{x_s}{L}\right) \frac{x_s}{L} \\
 \Rightarrow \sigma &= 1 - 3 \frac{x_s}{L} + 3 \left(\frac{x_s}{L}\right)^2
 \end{aligned}$$

and

$$\begin{aligned}
 \bar{\Delta}_3(L) &= \frac{\int_0^1 \sigma(x_s, L) dx_s}{1} \\
 &= \int_0^L \sigma(x_s, L) dx_s \\
 &= \frac{L}{15}
 \end{aligned} \tag{B.38}$$

For random spectra, no correlation exists between two different levels, and it turns out that $\bar{\Delta}_3 = \frac{L}{15}$ for all L .

Secondly, I calculate $\bar{\Delta}_3$ for the harmonic oscillator: $E_n = n$. Because of the periodicity of the spectrum, $\bar{\Delta}_3$ is

$$\bar{\Delta}_3(L) = \int_0^1 \sigma(E, L) dE$$

The sums from (B.36) can be calculated for integer L :

$$\begin{aligned}
 J(E, L) &= \frac{1}{3}L^2 + \left(E - \frac{1}{2}\right)L + \frac{1}{6} \\
 R(E, L) &= \frac{1}{2}L + \left(E - \frac{1}{2}\right) \\
 C(E, L) &= \frac{1}{6}L + \left(E - \frac{1}{6} - E^2\right)L^{-1}
 \end{aligned}$$

giving

$$\sigma(E, L) = \frac{1}{12} - 3\left(E - \frac{1}{6} - E^2\right)^2 L^{-2}$$

and

$$\bar{\Delta}_3(L) = \frac{1}{12} - \frac{1}{60L^2} \quad (\text{B.39})$$

Note that $\bar{\Delta}_3(1) = \frac{1}{15}$, in accordance with the result for small L . For L large, $\bar{\Delta}_3$ becomes constant. This is called *saturation*. Saturation should take place in all regular spectra, as I will argue in a moment, but I first mention the results for chaotic spectra, according to Random Matrix Theory[20]

$$\begin{aligned} \bar{\Delta}_3(L) &= \frac{1}{\pi^2} \left[\ln(2\pi L) + \gamma - \frac{\pi^2}{8} - \frac{5}{4} \right] && \text{for GOE} \\ \bar{\Delta}_3(L) &= \frac{1}{2\pi^2} \left[\ln(2\pi L) + \gamma - \frac{5}{4} \right] && \text{for GUE} \end{aligned}$$

where γ is Euler's constant.

I will now argue why a regular spectrum should have a saturating $\bar{\Delta}_3$. I start out with a one-dimensional regular spectrum $E_n = f(n)$. $\bar{\Delta}_3$ is usually calculated for a finite interval $[E_1, E_2]$, since for general $f(n)$ this has to be done numerically. If $f(n)$ is monotonous, unfolding would give $\{n\}$ as a spectrum and $\bar{\Delta}_3$ would saturate. But I will not unfold this spectrum at this moment, and concentrate on $\bar{\Delta}_3$ according to (B.36), for $E_n = f(n)$. For L not too large, the eigenvalues are approximately

$$E_n \approx f(E) + (n - E)f'(E)$$

which is like the harmonic oscillator, therefore $\bar{\Delta}_3$ will saturate, but the saturation point and the saturation value depend on how much of the eigenvalues are included.

Now look at a systems of which the spectrum is composed of two different spectra: $\{E_i\} = \{E_i^{(1)}\} \cup \{E_i^{(2)}\}$ ¹. $\sigma(E, L)$ contains just a sums over the energies, so the R , J and C from (B.36) are the sums of those quantities for the partial spectra 1 and 2. Since they are positive, I can deduce

$$\begin{aligned} \sigma &= J^{(1)} + J^{(2)} - (R^{(1)} + R^{(2)})^2 - 3(C^{(1)} + C^{(2)})^2 \\ &\leq J^{(1)} + J^{(2)} - (R^{(1)})^2 - (R^{(2)})^2 - 3(C^{(1)})^2 - (C^{(2)})^2 \\ &= \sigma^{(1)} + \sigma^{(2)} \end{aligned}$$

and so

$$\bar{\Delta}_3(L) \leq \bar{\Delta}_3^{(1)}(L) + \bar{\Delta}_3^{(2)}(L) \quad (\text{B.40})$$

Note that if the whole spectrum is unfolded, the partial spectra aren't. If the $\bar{\Delta}_3^{(1)}$ and $\bar{\Delta}_3^{(2)}$ are bounded from above, then $\bar{\Delta}_3$ is also bounded from above: it

¹Not $E_i = E_i^{(1)} + E_j^{(2)}$!

saturates if $\bar{\Delta}_3^{(1)}$ and $\bar{\Delta}_3^{(2)}$ saturate. Of course this can be generalized to spectra containing more than two saturating partial spectra.

Now look at a regular spectrum $E_{n_1, n_2, \dots, n_k} = f(n_1, n_2, \dots, n_k)$. I can split this spectrum into partial spectra as follows

$$\begin{aligned} \{f(n_1, n_2, n_3, \dots, n_k)\} &= \{f(n_1, 1, \dots, 1)\}_{n_1 > 0} \cup \{f(1, n_2, \dots, 1)\}_{n_2 > 1} \dots \cup \{f(1, 1, \dots, n_k)\}_{n_k > 1} \\ &\cup \{f(n_1, 2, \dots, 2)\}_{n_1 > 1} \cup \{f(2, n_2, \dots, 2)\}_{n_2 > 2} \dots \cup \{f(2, 2, \dots, n_k)\}_{n_k > 2} \\ &\cup \{f(n_1, 3, \dots, 3)\}_{n_1 > 2} \cup \{f(3, n_2, \dots, 3)\}_{n_2 > 3} \dots \cup \{f(3, 3, \dots, n_k)\}_{n_k > 3} \\ &\vdots \end{aligned} \tag{B.41}$$

The restrictions are necessary so that every level occurs only once in the right hand side. As I saw, each of these partial spectra saturate, so the whole spectrum has to have a saturating $\bar{\Delta}_3$. The saturations points will have in general different values, so many saturation points exist. At such a point L^* , one will see that the slope decreases rather suddenly. If the rest of the partial spectra are still very much random on a scale L^* , $\bar{\Delta}_3$ will be almost linear. The graph of $\bar{\Delta}_3$ will therefore be composed of linear parts, with changes of the slope at saturation points. Generally, there are infinitely many of these points, the linear parts are probably not distinguishable. But if the spectrum is of the form $E_{n_1, n_2, \dots, n_k} = f_1(n_1) + f_2(n_2) + \dots + f_n(n_k)$, then the levels in every column behave the same, e.g. like $E_n \approx f_1(n_1) + f_2(E) + \dots + f_n(n_k) + f'_2(E)(n_2 - E)$ for the second column. Thus the whole column will have roughly the same saturation point. The whole spectrum can then have maximally clear k saturation points, where k was the number of quantum numbers. In between these point, $\bar{\Delta}_3$ will be approximately linear, and at these point the slope decreases suddenly. At the last saturation point, total saturation takes place.

C Technical Results

C.1 Continuity of Characteristic Curves

In this section the following theorem will be proved

Theorem C.1 *Consider a Sturm-Liouville problem*

$$\left[\frac{\partial}{\partial x} p(x) \frac{\partial}{\partial x} + \lambda R(x) + \xi K(x) + S(x) \right] y(x) = 0 \tag{C.1}$$

with p positive, continuous differentiable, R , S and K continuous, R positive, and with certain boundary conditions imposed. If there exist a constant c such that $cK(x) < R(x)$, then the characteristic curves $\lambda_k(\xi)$ are continuous functions of ξ .

I already saw in section 2.1.6 that the characteristic curves are at least piecewise continuous. Discontinuities of these curves can be shown not to exist when the restriction is imposed on $K(x)$, as I will show now. All combinations (ξ, λ) for which (2.60) with boundary conditions has a solution are given by the characteristic curves. Note that these curves have an "intrinsic" numbering k from

1 to infinity, corresponding to the number of zero's of the solution y , and that $\lambda_k(\xi)$ has a value for all ξ s: it a function of ξ . Now perform a rotation in the (ξ, λ) plane,

$$\begin{aligned}\xi' &= \xi \cos \phi + \lambda \sin \phi \\ \lambda' &= -\xi \sin \phi + \lambda \cos \phi\end{aligned}\tag{C.2}$$

which transforms (2.60) to

$$\left[\frac{\partial}{\partial x} p(x) \frac{\partial}{\partial x} + \lambda' [R(x) \cos \phi - K(x) \sin \phi] + \xi' [K(x) \cos \phi + R(x) \sin \phi] + S(x) \right] y(x) = 0$$

or

$$\left[\frac{\partial}{\partial x} p(x) \frac{\partial}{\partial x} + \lambda' R'(x) + \xi' K'(x) + S(x) \right] y(x) = 0\tag{C.3}$$

where

$$R'(x) = R(x) \cos \phi - K(x) \sin \phi\tag{C.4}$$

$$K'(x) = K(x) \cos \phi + R(x) \sin \phi\tag{C.5}$$

Since the problem isn't changed, all the pairs (ξ', λ') for which the boundary value problem has a solution is given by the same, rotated, characteristic curves as (2.60):

$$\{(\xi', \lambda')\} = \{(\xi \cos \phi + \lambda_k(\xi) \sin \phi, -\xi \sin \phi + \lambda_k(\xi) \cos \phi)\}\tag{C.6}$$

If I suppose for now that $R'(x) > 0$ for all $a \leq x \leq b$, then again these pairs form a set of piecewise continuous functions

$$\{(\xi', \lambda')\} = \{(\xi', \lambda'_k(\xi'))\}\tag{C.7}$$

Since k counts the number of zero's of y , which isn't changed, the indices k on λ' coincide with those on λ :

$$(\xi', \lambda'_k(\xi')) = (\xi \cos \phi + \lambda_k(\xi) \sin \phi, -\xi \sin \phi + \lambda_k(\xi) \cos \phi)\tag{C.8}$$

which means that the λ part of the right hand side can be expressed in the ξ part. Now I need the following proposition

Proposition C.1 *Let C be a piecewise continuous curve in R^2 that is the graph of a finite function $y_c(x)$ in a coordinate frame (x, y) . If there exists a $\phi \neq 0$ such that under a rotation over an angle ϕ of the coordinate frame, C is again the graph of a finite function $y'_c(x')$ then C is everywhere continuous.*

Proof: First I'll prove that the discontinuous jumps in $y_c(x)$ and $y'_c(x)$ can only be in one direction: either the right limit is larger than the left limit on all these points, or the otherway around. This is seen easily, since if jumps in different directions occurred, under the rotation over ϕ , one of these jumps induces a multi-valuedness of $y'_c(x')$, as is shown in figure 35. Now I look at an

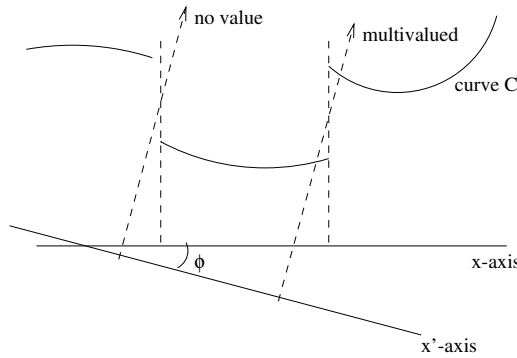


Figure 35: Multivaluedness of y'_c when jumps in y_c are not unidirectional

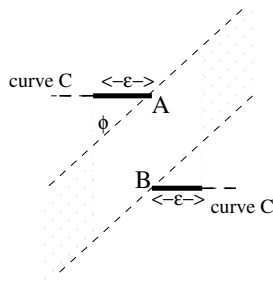


Figure 36: Options for the missing part of the graph of y'_c

arbitrary jump. Under rotation a part of the function y'_c seems to be missing. Since y_c is continuous in a left neighborhood, of size $\epsilon > 0$ say, and in a right neighborhood of the jump and single-valued, the missing part of C has to lie in the shaded areas of figure 36. This would mean that the graph of y'_c would have to make a jump downwards from A first to the lower shaded area and then a jump back upwards to B , or first jump to the upper shaded area and then jump back. In any case, these jump are in different directions, which was not possible: I get a contradiction and have to conclude that C cannot have discontinuities. \square

So I see that the characteristic curves are continuous provided that $R'(x) > 0$ for some nonzero ϕ . For not to large ϕ , $\cos \phi$ is positive, and $\sin \phi$ is small. If $K(x)$ does not blow up with respect to $R(x)$, which was positive to start with, then there is always a ϕ such that $R'(x)$ is positive for all x . More precisely, there should exist a constant c , such that

$$cK(x) < R(x) \tag{C.9}$$

where c is allowed to be negative. If c is positive, I can choose ϕ positive and smaller than $\arctan c$, so

$$\begin{aligned} R'(x) &= \cos \phi [R(x) - K(x) \tan \phi] \\ &> \cos \phi [R(x) - R(x)/c \tan \phi] \\ &= \cos \phi R(x) [1 - 1/c \tan \phi] \\ &> 0 \end{aligned}$$

If c is negative, ϕ can be chosen negative and larger than $\arctan c$, then in the same manner one finds $R'(x) > 0$. This completes the proof of the theorem.

C.2 Laplace Operator in Arbitrary Coordinates

I will now calculate the Laplacian in an arbitrary coordinate system. Starting from Cartesian coordinates (x_1, x_2) :

$$\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}$$

I perform a coordinate transformation to (z, θ)

$$\begin{aligned} x_1 &= x_1(z, \theta) \\ x_2 &= x_2(z, \theta) \end{aligned}$$

The Jacobian-matrix of this transformation is

$$J = \begin{pmatrix} \frac{\partial x_1}{\partial z} & \frac{\partial x_1}{\partial \theta} \\ \frac{\partial x_2}{\partial z} & \frac{\partial x_2}{\partial \theta} \end{pmatrix} \quad (\text{C.10})$$

In the following, I will use Einsteins summation convention, where indices take the values 1 and 2. Denoting $(\partial_1, \partial_2) = (\frac{\partial}{\partial z}, \frac{\partial}{\partial \theta})$, the gradient becomes

$$\frac{\partial}{\partial x_i} = (J^{-1})_{ji} \partial_j$$

Since

$$\Delta = \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_i}$$

I get

$$\begin{aligned} \Delta &= J_{ji}^{-1} \partial_j J_{ki}^{-1} \partial_k \\ &= J_{ji}^{-1} J_{ki}^{-1} \partial_j \partial_k + J_{ji}^{-1} (\partial_j J_{ki}^{-1}) \partial_k \end{aligned}$$

Using

$$\begin{aligned} \partial_i (J_{ij}^{-1}) J_{jk} + J_{ij}^{-1} \partial_i (J_{jk}) &= \partial_i (J_{ij}^{-1} J_{jk}) \\ &= \partial_i \delta_{ik} \\ &= 0 \end{aligned}$$

I finally get

$$\begin{aligned} \Delta &= J_{ji}^{-1} J_{ki}^{-1} \partial_j \partial_k - J_{ji}^{-1} J_{li}^{-1} (\partial_j J_{ml}) J_{km}^{-1} \partial_k \\ &= (J^T J)_{jk}^{-1} \left[\partial_j \partial_k - (\partial_j J_{mk}) J_{lm}^{-1} \partial_l \right] \end{aligned} \quad (\text{C.11})$$

C.3 Standard Hamiltonian in Arbitrary Coordinates

The standard Hamiltonian in two dimensions

$$\mathcal{H} = \frac{|\vec{p}|^2}{2m} + V(x)$$

will be transformed to an arbitrary coordinate system. The Lagrangian is

$$L = \frac{1}{2}m |\dot{\vec{x}}|^2 - V(\vec{x})$$

I perform a coordinate transformation from $\vec{x} = (x_1, x_2)$ to $\vec{z} = (z, \theta)$

$$\begin{aligned} x_1 &= x_1(z, \theta) \\ x_2 &= x_2(z, \theta) \end{aligned}$$

The Jacobian-matrix of this transformation is

$$J = \begin{pmatrix} \frac{\partial x_1}{\partial z} & \frac{\partial x_1}{\partial \theta} \\ \frac{\partial x_2}{\partial z} & \frac{\partial x_2}{\partial \theta} \end{pmatrix} \quad (\text{C.12})$$

so $\dot{\vec{x}} = J\dot{\vec{z}}$ and

$$|\dot{\vec{x}}|^2 = \dot{z}_i (J^T J)_{jk} \dot{z}_k \quad (\text{C.13})$$

The generalized momenta associated with \vec{z} are then

$$\vec{p}' = m(J^T J)\dot{\vec{z}} \quad (\text{C.14})$$

The kinetic term thus becomes

$$T = \frac{p'_i (J^T J)_{ij} p'_j}{2m}$$

and the Hamiltonian is

$$\mathcal{H} = \frac{p'_i (J^T J)_{ij} p'_j}{2m} + V(\vec{z}) \quad (\text{C.15})$$

C.4 Asymptotic Behavior of $a(q)$

I will now give a derivation of the result in (2.70). The proof can also be found in Arscott[2]. Look at (2.65), but now write $x = 2\sqrt{k}(z - \pi/2)$ and $w(x, k) = y(z, q)$ then

$$\frac{d^2 w}{dx^2} + \left[\lambda(k) - k \sin^2 \left(\frac{x}{2\sqrt{k}} \right) \right] w = 0 \quad (\text{C.16})$$

where

$$\begin{aligned} \lambda(k) &= \frac{a + 2k^2}{4k} \\ &= \beta/4 \end{aligned}$$

For ce_{2n} boundary conditions become

$$\begin{aligned} w(0) &= 1 \text{ (when suitably normalized)} \\ w'(0) &= w'(\pm\pi\sqrt{k}) \\ &= 0 \end{aligned}$$

The proof is similar for ce_{2n+1} and se_m . I need the following proposition

Proposition C.2 *If y is any continuous non-zero solution of an equation of the form $y'' + f(x)y = 0$, and if for $a \leq x \leq b$, $f(x) < 0$, then there can be at most one zero of the product yy' in $[a, b]$, that is, one zero of y or one zero of y' .*

Note that w has n zero's in $[0, \pi\sqrt{k}]$. Now let $I_1 = [0, \pi\sqrt{k}]$ and $I_2 \subset I_1$ such that $\lambda(k) > k \sin^2(\frac{x}{2\sqrt{k}})$. Then according to the proposition, the part of I_1 outside of I_2 contains at most one zero of y or y' . Now for an x in I_2 :

$$\sin^2 \frac{x}{2\sqrt{k}} < \frac{\lambda(k)}{k}$$

With $\sin \theta > \theta - \theta^3/6$ for $\theta < \sqrt{6}$ and $x \leq \pi\sqrt{k}$, I get

$$\frac{x^2}{4} \left(1 - \frac{\pi^2}{24}\right)^2 \leq \lambda(k) \quad (\text{C.17})$$

Now $\lambda(k)$ is finite, so I_2 is a finite interval. Thus, for k large enough, $x = \pi\sqrt{k}$ is outside of I_2 . I know that $w'(\pi\sqrt{k}) = 0$, so all zero's of $w(x)$ are in I_2 and all zero's of $w'(x)$ – except the one at $x = \pi\sqrt{k}$ – in I_2 . Then the absolute maximum of w in I_1 is also in I_2 . Now I take $k \rightarrow \infty$, and call $w(x, k \rightarrow \infty) = v(x)$, and get

$$\frac{d^2v}{dx^2} + \left(l - \frac{x^2}{4}\right)v = 0 \quad (\text{C.18})$$

with the conditions

- $v(0) = 1$ and $v'(0) = 0$,
- v is finite at infinity,
- $v(x)$ has n (simple) poles in $0 < x < \infty$

This is just the equation for a harmonic oscillator, with $\hbar\omega = 1$. The eigenvalues l would thus be $n + \frac{1}{2}$, but the first condition picks out the even solutions around the origin, corresponding to even values of n , so I am left with $l = 2n + \frac{1}{2}$. Thus

$$\frac{\beta}{4} = \lambda(k) \sim l = 2n + \frac{1}{2} = m + \frac{1}{2}$$

for ce_m , and

$$\frac{a + 2q}{\sqrt{q}} \sim 4\left(m + \frac{1}{2}\right) \quad (\text{C.19})$$

and (2.70) follows.

C.5 The Integrals I_n and L_n

In the asymptotic approach, certain integrals emerged. I will take a closer look at them here. The integrals are defined up to an additional constant by

$$L_n(z) \equiv \int^z \frac{dz'}{\cos^n z'} \quad (\text{C.20})$$

and

$$\begin{aligned} I_n(z) &\equiv \int^z \frac{\sin z'}{\cos^n z'} dz' \\ &= \frac{1}{(n-1) \cos^{n-1} z} \end{aligned} \quad (\text{C.21})$$

For the L_n a recursion relation can be obtained:

$$L_{n+2}(z) = \frac{1}{n+1} \left[\frac{\sin z}{\cos^{n+1} z} + nL_n(z) \right] \quad (\text{C.22})$$

which can be checked by differentiation. The constant that would remain to be determined is defined by (C.22) to be the same for all L_n , since (C.20) only defined L_n up to a constant any way. The recursion relation terminates at L_1 or L_2 :

$$\begin{aligned} L_1(z) &= \int^z \frac{1}{\cos z'} dz' \\ &= \log \tan\left(\frac{z}{2} + \frac{\pi}{4}\right) \end{aligned} \quad (\text{C.23})$$

$$\begin{aligned} L_2(z) &= \int^2 \frac{1}{\cos^2 z'} dz' \\ &= \frac{\sin z}{\cos z} \end{aligned} \quad (\text{C.24})$$

Which further sets the constant of integration. Only L_n with n odd appear in the asymptotic method. One sees that all L_n with n odd, contain a *logarithmic* term L_1 . This makes the asymptotic approach possible.

C.6 Hermiticity in Arbitrary Coordinates

I wish to give some attention to hermiticity of the operators constructed in section 3.1.1. In order that these quantities can represent real observables, they have to be hermitian. The original Schrödinger equation might have been obtained by some coordinate transformation. This affects the hermiticity of differential operators, since hermiticity is now to be interpreted with respect to the inner product

$$\langle \Psi | \Phi \rangle = \iint R(z, \theta) \Psi^*(z, \theta) \Phi(z, \theta) dz d\theta \quad (\text{C.25})$$

where $R(z, \theta)$ is the Jacobian of the coordinate transformation, so it is a positive function of z and θ . This function may at this point seem to introduce more

arbitrariness into the system, but the requirement that \mathcal{H} be hermitian, will give a connection between R and M . Taking the conjugate of (3.5) will return \mathcal{H} again if

$$\begin{aligned} D_z^\dagger \frac{1}{M(z, \theta)} &= \frac{1}{M(z, \theta)} D_z \\ D_\theta^\dagger \frac{1}{M(z, \theta)} &= \frac{1}{M(z, \theta)} D_\theta \end{aligned}$$

multiplying both sides with M gives me

$$\begin{aligned} M(z, \theta) D_z^\dagger &= D_z M(z, \theta) \\ M(z, \theta) D_\theta^\dagger &= D_\theta M(z, \theta) \end{aligned} \tag{C.26}$$

hermitian conjugates of a differential operator are usually found by performing a partial integration. In (C.25), R will then also be differentiated. In this way, I find¹

$$\begin{aligned} \left(\frac{\hbar}{i} \frac{\partial}{\partial z}\right)^\dagger &= \frac{\hbar}{i} \frac{\partial}{\partial z} + \frac{\hbar}{i} \frac{\partial \log R}{\partial z} \\ \left(\frac{\hbar}{i} \frac{\partial}{\partial \theta}\right)^\dagger &= \frac{\hbar}{i} \frac{\partial}{\partial \theta} + \frac{\hbar}{i} \frac{\partial \log R}{\partial \theta} \end{aligned} \tag{C.27}$$

and

$$\begin{aligned} \left(\frac{\partial^2}{\partial z^2}\right)^\dagger &= \frac{\partial^2}{\partial z^2} + \left(\frac{\partial \log R}{\partial z}\right)^2 + 2 \frac{\partial \log R}{\partial z} \frac{\partial}{\partial z} + \frac{\partial^2 \log R}{\partial z^2} \\ \left(\frac{\partial^2}{\partial \theta^2}\right)^\dagger &= \frac{\partial^2}{\partial \theta^2} + \left(\frac{\partial \log R}{\partial \theta}\right)^2 + 2 \frac{\partial \log R}{\partial \theta} \frac{\partial}{\partial \theta} + \frac{\partial^2 \log R}{\partial \theta^2} \end{aligned} \tag{C.28}$$

Substituting (3.3) into (C.26), using this last result, gives me

$$\begin{aligned} \frac{\partial \log M}{\partial z} &= \frac{\partial \log R}{\partial z} \\ \frac{\partial \log M}{\partial \theta} &= \frac{\partial \log R}{\partial \theta} \end{aligned} \tag{C.29}$$

so that

$$\log M(z, \theta) = \log cR(z, \theta)$$

with c a constant. This constant can be set by an appropriate scaling. Such uniform scaling again doesn't influence the form of a billiard, so I may use $c = 1$. This sets the relative units of M and R which were undefined until now. It can be shown that Z is now also hermitian.

¹taking a logarithm might cause problems regarding units, but since only derivatives are involved, one it to understand that $\log X$ means $\log X/X_0$ where X_0 is an (arbitrary) unit of X .

D Numerical Methods

D.1 Runge-Kutta Method

In general one wishes to know the time-evolution of a vector \vec{y} , which is governed by the differential equation

$$\dot{\vec{y}} = \vec{f}(t, \vec{y}) \quad (\text{D.1})$$

To calculate from \vec{y}_n the value \vec{y}_{n+1} an interval h later, I could use something like

$$x(t+h) \leftarrow x(t) + hf(t) \quad (\text{D.2})$$

This is just Euler's method. In this form, it is not very accurate compared to other methods nor very stable. Several improvements are possible, such as increasing the order of the Taylor-approximation, but I do not wish to keep track of all the derivatives. Fortunately, I don't have too. There is a general strategy in which one takes trial-points between \vec{y}_n and \vec{y}_{n+1} , calculate \vec{f} there, and use some linear combination such that several error-terms cancel out, to find \vec{y}_{n+1} up to some order of h . This method is called the Runge-Kutta method. To make this more concrete, let me mention some cases. First, the Runge-Kutta method up to an accuracy of the order of h^1 reduces to the Euler method (D.2). Furthermore, the form of the fourth order Runge-Kutta method, which will show some of the general appearance of the method, looks like[19]

$$\begin{aligned} \vec{k}_1 &\leftarrow h \vec{f}(t, \vec{y}_n) \\ \vec{k}_2 &\leftarrow h \vec{f}\left(t + \frac{h}{2}, \vec{y}_n + \frac{\vec{k}_1}{2}\right) \\ \vec{k}_3 &\leftarrow h \vec{f}\left(t + \frac{h}{2}, \vec{y}_n + \frac{\vec{k}_2}{2}\right) \\ \vec{k}_4 &\leftarrow h \vec{f}(t+h, \vec{y}_n + \vec{k}_3) \\ \vec{y}_{n+1} &\leftarrow \vec{y}_n + \frac{\vec{k}_1}{6} + \frac{\vec{k}_2}{3} + \frac{\vec{k}_3}{3} + \frac{\vec{k}_4}{6} \end{aligned} \quad (\text{D.3})$$

The exact answer for \vec{y}_{n+1} differs only by a term of order h^5 . It is possible to further enhance the Runge-Kutta method by adjusting the step-size h to some required accuracy while running the algorithm. At first I thought I would have to use this in my calculations too since I have a very big increment in a very small area (the edge of the ellipse), so the numerical solutions might jump over it. This was not necessary however. In my implementation, I wanted to directly plot the trajectory (using (1.1)) for several reasons. I wouldn't have to store the calculated path, I could see if any errors were made, I would be able to stop the calculation when I think it has gone far enough to give the right impression. Such an impression is best achieved if the time step h is constant. Then I could also get some idea of the velocity of the particle. It turned out that the algorithm (D.3) was enough to get the solution of the particle with good accuracy, even near the edge for h small enough, within a acceptable

time (in the order of minutes). A particle could jump out the accessible region (the elliptical box in this case) due to a computational effect, but this would be visible immediately on the computer-screen by one of the following phenomena:

1. The particle crossed the boundary with a change of the direction of the velocity,
2. The particle is bounced back but at a notably higher speed than it had before.

Both effects can be explain by the – virtual – increase in energy the particle gets when it is pushed into the kinematically prohibited area. In case 2 the increase is still not enough to penetrate the wall further and therefore it manifests itself as an increase in kinetic energy. In case 1, the particle apparently jumped into a flat part of the potential (see section 1.2), so it doesn't fall back. Since the influence in one direction is different from that in the other, the direction of the velocity changes. When one of these phenomena occurred, I could simply stop the program, increase the number of steps per second – lowering the value of h – to fix the problem.

D.2 Diagonalization Method

The diagonalization method used is taken from Numerical Recipes[19]. It consists of two steps

- First the matrix is reduced to tri-diagonal form (non-zero element only on the diagonal and sub/superdiagonals), using the Householder-method. This means that one performs so-called Householder transformations on the matrix, which are constructed such that they zero all elements of a column below the subdiagonal. The transformations are orthogonal, and preserve symmetry. Performing $n - 1$ of these transformations thus leaves the matrix in tridiagonal form.
- Next, this tridiagonal matrix is diagonalized, using the so-called QL-algorithm, which consists of the following. Any real matrix A can be written in the form

$$A = QL$$

where L is lower triangular and Q is orthogonal. The QL algorithm now consists of a sequence of orthonormal transformations:

$$A_s = Q_s L_s \rightarrow A_{s+1} = L_s Q_s = Q_s^T A_s Q_s$$

There is a theorem that states that A_s will converge to lower triangular form, except for degenerate eigenvalues. Then a diagonal block appears in A_s , of size p if p is the multiplicity of the eigenvalue. This means that when A is symmetric, all the A_s are, and A_s converges to diagonal form. If there are p times degenerate eigenvalues, at least $p - 1$ zero's should occur on the sub-diagonal, and the matrix can be split into two matrices that can be

diagonalized separately. The calculated eigenvalues thus can not influence each other: the method is not particularly unstable for degenerate levels. Several techniques are possible to optimize the methods, as explained in [19]. The method is only applicable for tridiagonal matrices, for full matrices the workload would get to big ($\mathcal{O}(n^3)$).

D.3 Sturm-Liouville Eigenvalue Problems

One dimensional eigenvalue problems like (2.60) give rise to tridiagonal matrices when the interval $[x_1, x_2]$ is discretized, so a numerical diagonalization using the QL-algorithm of the previous section is possible. Discretization is done as follows. Take n equally spaced points in the interior of the interval. The spacing is $\Delta x = \frac{x_2-x_1}{n+1}$. Call $y(i\Delta x) = y_i$, and define

$$\begin{aligned} D_r y_i &= \frac{1}{\Delta x} [y_{i+1} - y_i] \\ D_l y_i &= \frac{1}{\Delta x} [y_i - y_{i-1}] \end{aligned}$$

Then $\frac{\partial}{\partial x} p(x) \frac{\partial}{\partial x} y$ can be discretized by

$$\frac{1}{\Delta x} \left\{ p\left(x + \frac{\Delta x}{2}\right) D_r - p\left(x - \frac{\Delta x}{2}\right) D_l \right\} y_i$$

All other terms in (2.60) give diagonal contributions. Boundary conditions can be implemented using $y_0 = 0$ and $y_{n+1} = 0$ for Dirichlet conditions or $D_l y_1 = 0$ and $D_r y_n$ for Neumann conditions. Finally, a multiplication with $R^{-\frac{1}{2}}$ on both sides in necessary, analogous to (2.55). The resulting matrix looks like

$$\left(\begin{array}{ccc} \frac{\frac{1}{\Delta x^2} \left\{ p\left(\frac{\Delta x}{2}\right) - p\left(\frac{3\Delta x}{2}\right) \right\} - \xi K(\Delta x) - S(\Delta x)}{R(\Delta x)} & \frac{p\left(\frac{3\Delta x}{2}\right)}{\Delta x^2 \sqrt{R(\Delta x)R(2\Delta x)}} & 0 \quad \dots \\ & & \ddots \\ \frac{p\left(\frac{3\Delta x}{2}\right)}{\Delta x^2 \sqrt{R(\Delta x)R(2\Delta x)}} & \frac{\frac{1}{\Delta x^2} \left\{ p\left(\frac{3\Delta x}{2}\right) - p\left(\frac{5\Delta x}{2}\right) \right\} - \xi K(2\Delta x) - S(2\Delta x)}{R(2\Delta x)} & \\ 0 & \ddots & \ddots \\ \vdots & & \end{array} \right)$$

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