TÉCNICO LISBOA

Applications of the Wigner function to quantum problems involving angle variables

Luís Miguel da Silva Pereira

Thesis to obtain the Master of Science Degree in

Engineering Physics

Supervisors: Prof. João Pedro Saraiva Bizarro
Prof. Hugo Fernando Santos Terças

Examination Committee

Chairperson: Prof. Luís Paulo da Mota Capitão Lemos Alves
Supervisor: Prof. Hugo Fernando Santos Terças
Member of the Committee: Prof. António Carlos Almeida Figueiredo

June 2022

Declaração

Declaro que o presente documento é um trabalho original da minha autoria e que cumpre todos os requisitos do Código de Conduta e Boas Práticas da Universidade de Lisboa.

Declaration

I declare that this document is an original work of my own authorship and that it fulfills all the requirements of the Code of Conduct and Good Practices of the University of Lisbon.

In memoriam João Pedro

Acknowledgments

During the main part of the research presented in this thesis I benefitted from an Initiation to Research Fellowship at the Instituto de Plasmas e Fusão Nuclear. This fellowship was vital, without it this work would never have been done.

Professor João Pedro Bizarro was the mentor of this work. He gave me the starting point from which everything else followed. He was also instrumental in procuring the fellowship from IPFN. I deeply appreciate the time we spent together.

After the passing away of Professor Bizarro, Professor Hugo Terças agreed to be my advisor so that I could finish the Physics Master's degree. I thank him very much for his availability and patience.

During this research I talked with several people about some of the aspects of this work. I thank especially José Agapito Ruiz, Vítor Rocha Vieira, Bruno Dinis and Pedro Freitas for stimulating conversations that were fundamental to the development of several parts of this thesis.

The support of my family, financial and otherwise, was fundamental for this work. I thank them for not stopping to believe in me.

Resumo

Nesta tese é estudado o modelo do Pêndulo Quântico na representação da função de Wigner e na representação do Operador de Densidade. Com vista a isto um modelo auxiliar completamente resolúvel é introduzido. Várias famílias de soluções das equações de estacionaridade são encontradas e comparadas. A vantagem da utilização da função de Wigner na descoberta de soluções é tornada evidente. Uma abordagem mais simples para a derivação das equações de evolução é desenvolvida. Ligações com as funções de Mathieu e a equação de Helmholtz da física-matemática clássica são analisadas.

Palavras-chave: função de Wigner, operador de densidade, pêndulo quântico, funções de Mathieu, equação de Helmholtz

Abstract

In this thesis the model of the Quantum Pendulum is studied in the Wigner function representation and in the Density Operator representation. Towards this end a completely solvable auxiliary model is introduced. Several families of solutions of the stationarity equations are found and compared. The advantage of using the Wigner function in the discovery of these solutions is made evident. A simpler approach to the derivation of the evolution equations is developed. Links with Mathieu functions and the Helmholtz equation of classical mathematical-physics are analized.

Keywords: Wigner function, density operator, quantum pendulum, Mathieu functions, Helmholtz equation

Contents

List of Acronyms and Symbols

Acronyms

SHR	Simplified Hindered Rotator	$\hat{H} = \omega \hat{l} - \lambda \cos(\hat{\theta})$
QP	Quantum Pendulum	$\hat{H} = \frac{\hat{l}^2}{2I} - \lambda \cos(\hat{\theta})$

Symbols

c	coupling constant of the Simplified Hindered Rotator	$c = -\frac{\lambda}{2\hbar\omega}$
c	coupling constant of the Quantum Pendulum	$c = -\frac{\lambda I}{\hbar^2}$
q	parameter of Mathieu equation	$q = -\frac{4\lambda I}{\hbar^2} = 4c$
Ω	parameter of Helmholtz 2d equation	$\Omega^2 = -\frac{16\lambda I}{\hbar^2} = 16c$
y	variable associated to Simplified Hindered Rotator	$y = 2\frac{\lambda}{\hbar\omega}\cos(\theta)$ $= -4c\cos(\theta)$
y	variable associated to Quantum Pendulum	$y = -2\frac{\lambda I}{\hbar^2}\cos(\theta)$ $= 2c\cos(\theta)$
$J_n(z)$	Bessel function of index n	
$a_{m,n}$	Fourier coefficient of Wigner transform	
MT	Mellin transform	

Chapter 1

Introduction

When I first enrolled in the Physics degree I also bought Nik Weaver's *Mathematical Quantization*. As the reader can gather from its title, it's a math book. It is an introduction to C^*-algebras, von Neumann-algebras and to Quantum Kinematics seen from the point of view of those operator algebras. In the book the author presents Bopp operators and the Weyl map, although the former not by name and the latter only via Fourier transforms. I ended up never systematically studying the book, but I skimmed through it frequently. This was my first introduction to phase-space quantization without really knowing it.

A bit more than two years later I came across a paper by C. J. Fewster and H. Sahlmann on phase-space quantization in Loop Quantum Cosmology where the authors give a definition of the Wigner function for the Bohr compactification of the real line. I think that exploring the bibliography I possibly saw Prof. Bizarro's name for the first time. But, at the time I was far from realizing that he was Portuguese and moreover a professor at IST!

I eventually met Prof. Bizarro when he was in charge of the course on *Plasma Kinetic Theory*. At our first meeting he asked me what made me choose this optional course and I answered "the bibliography of the course" (I was interested in learning stochastic processes and N. G. van Kampen's book was in the secondary bibliography). We immediately liked each other. He was very pleased by my answer and henceforth would recommend to his colleagues to pay attention to the bibliography of their courses in the corresponding webpages. Since this course functioned in a tutorial regime, it was quite informal, so that one day Bizarro asked me if I had heard about phase-space quantization and the Wigner function and I said yes. We didn't follow through on this conversation, but he became interested in our future collaboration. This is how two years later I came to benefit from an Initiation to Research Fellowship from IPFN dedicated to the Wigner function for angular variables.

1.1 Motivation

My initial interest in this work was mostly as an excuse to study abstract Harmonic analysis. But, during the course of its execution I ended up not studying the kind of abstract mathematics I initially intended, but instead I studied special functions, difference equations, combinatorial identities, generating functions, computational commutative algebra, solving differential equations using symmetries, umbral calculus, the Mellin transform and complex analysis. I hardly think there is an area in mathematics more concrete than combinatorial identities. The thing that made me change my plans was the discovery in the first few weeks of research of explicit solutions to the stationarity equation for the Wigner function of the Quantum Pendulum. If these could be proven to be pure states then an explicit formula for Mathieu functions would probably follow. This is something that has been missing since their discovery in 1868 [1], more than 150 years ago, and one of the reasons why Mathieu functions have not reached the level of prominence of Bessel functions in applied mathematics.

What justified my obsession with this problem for the next two years was the similarity between the two difference-differential equations

$$2\frac{\partial Z}{\partial y}(y,m) = Z(y,m-1) - Z(y,m+1) \tag{1.1}$$

and

$$m\frac{\partial Z}{\partial y}(y,m) = Z(y,m+1) - Z(y,m-1). \tag{1.2}$$

The first is the equation for a solvable model that in this thesis will be called *Simplified Hindered Rotator* and the second is the one for the Quantum Pendulum. In his Ph.D. thesis [2], Bizarro observed that Bessel functions provide a solution to the first equation and he asked me to look at books to try to find a solution to the second equation. I ended up not doing exactly that, but instead I tried to rederive the expression for Bessel functions as power series from the first equation and adapt it to the second one. This worked the first time I tried!

It will be seen in this thesis that it is very easy to adapt derivations of solutions of the solvable model to obtain solutions of the Quantum Pendulum. But, the higher prize of discovering which of these solutions correspond to pure states and hence to Mathieu functions elluded me. It will be seen that none of the solutions derived for the Quantum Pendulum is a pure state, one must therefore make linear combinations of them to obtain pure states.

1.2 Brief review of the Wigner transform

From the wave function $|\psi\rangle$ describing a quantum system, Wigner [3] defined a function $W(x,p)$ in phase space that has the property that the marginal probabilities are the quantum probabilities:

$$\int_{-\infty}^{+\infty} dp\, W(x,p) = |\langle x|\psi\rangle|^2 = |\psi(x)|^2 \tag{1.3}$$

and

$$\int_{-\infty}^{+\infty} dx\, W(x,p) = |\langle p|\psi\rangle|^2 = |\tilde{\psi}(p)|^2, \tag{1.4}$$

where $\tilde{\psi}$ is the Fourier transform. There are an infinite number of functions with this property [4], yet the one defined by Wigner, namely,

$$\begin{aligned} W(x,p) &= \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dx' e^{\frac{i}{\hbar}px'} \langle x - \tfrac{x'}{2}|\psi\rangle\langle\psi|x + \tfrac{x'}{2}\rangle \\ &= \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dp' e^{\frac{i}{\hbar}p'x} \langle p + \tfrac{p'}{2}|\psi\rangle\langle\psi|p - \tfrac{p'}{2}\rangle. \end{aligned} \tag{1.5}$$

has a certain number of extra properties that make it unique [5, 6].

The above feature of the Wigner function might lead one to believe that Quantum Mechanics is then just a statistical theory. This is not the case, the main novelty is that now $W(x,p)$ can have negative values. This local negativity of the Wigner function is a new physical resource.

Trying to define an analogue of the Wigner function to deal with angle/angular-momentum variables, we have to deal with a new phenomenon, that of the quantization of the angular momentum, that is, the values of the angular momentum l no longer form a continuum, as in the standard position/momentum case, but their only allowed values are $l = m\hbar$, with m an integer. Therefore, the quantum phase space is no longer $\mathbb{R}^2$ as in the standard case, but the angle/angular-momentum pairs (θ, l) now live in $S^1 \times \hbar\mathbb{Z}$. Mathematically, this corresponds to the fact that the dual group of $\mathbb{R}$ is $\mathbb{R}$, but the dual group of S^1 is $\mathbb{Z}$ (implying, reciprocally, that the dual group of $\mathbb{Z}$ is S^1). For convenience, we will work with the phase space $S^1 \times \mathbb{Z}$ instead of $S^1 \times \hbar\mathbb{Z}$, and with pairs (θ, m) instead of (θ, l).

To deal with the rotational spectrum, Berry [7] defined the Wigner function

$$W(\theta,m) = \frac{1}{2\pi}\int_{-\pi}^{+\pi} d\theta' e^{im\theta'} \langle \theta - \tfrac{\theta'}{2}|\psi\rangle\langle\psi|\theta + \tfrac{\theta'}{2}\rangle, \tag{1.6}$$

which can also be found in Mukunda [8] and in Berman and Kolovsky [9]. With this expression one obtains the right marginals:

$$\sum_{m=-\infty}^{+\infty} W(\theta,m) = |\langle\theta|\psi\rangle|^2 \tag{1.7}$$

and

$$\int_{-\pi}^{+\pi} d\theta\, W(\theta,m) = |\langle m|\psi\rangle|^2. \tag{1.8}$$

The Wigner transform can be seen as a linear map from operators $\hat{A}$ to phase-space functions $A(\theta,m)$, with the Wigner function $W(\theta,m)$ corresponding to the density operator $\hat{\rho} = |\psi\rangle\langle\psi|$:

$$A(\theta,m) = \frac{1}{2\pi}\int_{-\pi}^{+\pi} d\theta' e^{im\theta'} \langle \theta - \tfrac{\theta'}{2}|\hat{A}|\theta + \tfrac{\theta'}{2}\rangle. \tag{1.9}$$

This leads immediately to the question of defining the correspondent of operator products $\hat{A}\cdot\hat{B}$ in terms of phase-space functions, the so-called Moyal product $A\bigstar B$, and the correspondent of the Lie bracket $[\hat{A},\hat{B}]$ for phase-space functions, called the Moyal bracket $[A,B]_\bigstar$. The differential form of the Moyal bracket in the standard position/momentum case, computed by Groenewold [10, 11], is actually simpler than the differential form of the Moyal product, due to cancelling of terms. The integral forms of the Moyal product and bracket, due to Baker [12], are similar, just substitute a complex exponential by a sine. The differential form can also be derived from an integral form involving the two-dimensional Fourier transforms of the Wigner transforms [6].

In the case of angle/angular-momentum variables no such formula is known, which led Bizarro [2] to define a new Wigner function for these variables in a manner such that the Moyal bracket could be computed, a modification that is best set down in the angular momentum basis and involves a doubling of points:

$$w(\theta,m)=\frac{1}{2\pi}\sum_{\substack{m' \text{ same} \\ \text{parity as } m}} e^{i\theta m'}\langle \tfrac{m+m'}{2}|\psi\rangle\langle\psi|\tfrac{m-m'}{2}\rangle. \tag{1.10}$$

This transform was first defined by Chan [13] in the context of signal processing, when looking for alias-free time-frequency representations of discrete-time signals [14]. Here we find preferable to work with even and odd integers, rather than with integer and semi-integers [2], so the points with physical meaning are those (θ, m) with m even, which correspond to the actual physical points $(\theta, m/2)$.

The marginal probabilities are given by:

$$\sum_{m=-\infty}^{+\infty} w(\theta,m)=|\langle\theta|\psi\rangle|^2 \tag{1.11}$$

and

$$\int_{-\pi}^{+\pi} d\theta\; w(\theta,m)=\begin{cases} |\langle\frac{m}{2}|\psi\rangle|^2 & \text{if } m \text{ even} \\ 0 & \text{if } m \text{ odd}\end{cases} \tag{1.12}$$

and, in the case of even angular momenta, there is a simple relation between the two Wigner functions:

$$w(\theta,2m)=\frac{W(\theta,m)+W(\theta+\pi,m)}{2}. \tag{1.13}$$

The marginal probability (1.11) can be further decomposed according to:

$$\sum_{m \text{ even}} w(\theta,m)=\frac{|\langle\theta|\psi\rangle|^2+|\langle\theta+\pi|\psi\rangle|^2}{2} \tag{1.14}$$

and

$$\sum_{m \text{ odd}} w(\theta,m)=\frac{|\langle\theta|\psi\rangle|^2-|\langle\theta+\pi|\psi\rangle|^2}{2}. \tag{1.15}$$

The modified Wigner transform (1.10) is immediately generalized to operators:

$$a(\theta,m)=\frac{1}{2\pi}\sum_{\substack{m' \text{ same} \\ \text{parity as } m}} e^{i\theta m'}\langle \tfrac{m+m'}{2}|\hat{A}|\tfrac{m-m'}{2}\rangle \tag{1.16}$$

and, while trying to obtain the evolution equation for the Wigner function, it was this modified Wigner transform that was used by Bizarro [2] to implicitly achieve formulas for the Moyal brackets. Alas, the formulas obtained in terms of operators acting on the coordinates θ and m are too complicated, which contrasts with the fact that the final results become quite simple when applied to specific phase space functions (check Eqs. (4.26) and (4.27) in [2], and compare with Eqs. (4.36) and (4.44) therein), the explanation for this resides in the simple form of the modified Wigner transform in the angular momentum basis, as will be seen in the next chapter.

1.3 The Wigner function in Plasma Physics

The focus of this thesis is in Quantum Mechanics, but it should be noted that the Wigner function also makes its appearance in Plasma Physics and, in particular, in the field of Fusion Plasmas. There are two main ways in which this happens. The first, through Classical Statistical Physics. The second through Signal Processing.

If Planck's constant h is set equal to zero, then the Moyal bracket becomes just the Poisson bracket. The evolution equation for the Wigner function then becomes the classical Liouville equation for the evolution of a probability density in phase space. Therefore, the evolution equation for the Wigner function can be seen as a generalization of the Liouville equation. A generalization with potentially infinitely many terms associated to increasing powers of a small parameter. This is actually how Bizarro first came to know about the Wigner function.

In the Kinetic theory of plasmas the $6N$ degrees of freedom associated to N particles are reduced to 6 degrees. In a Tokamak configuration, the three degrees associated to position are taken not from the usual three-dimensional Cartesian space $\mathbb{R}^3$, but from a $[0, R] \times \mathbb{T}^2$ compact space. Since now we have 2 angles it becomes interesting to formulate the Kinetic theory of angular variables. The Wigner function in this context can be seen from two perspectives. In the first, as an attempt to achieve a Kinetic equation. This is marred by the fact that it is natural for the Wigner function to have negative values. In the second perspective, one just considers Wigner transforms of wave functions defined in Tokamak configurations. Curiously, the difficulty in this context is to define a Wigner transform of the variable associated to the radius and not the angles. This is due to the fact that the radius is always a non-negative quantity.

The second way the Wigner function enters Fusion Plasmas is through Signal Processing, more specifically, Time-Frequency analysis. The Wigner transform is well-known in Time-Frequency analysis [4]. If one takes the variable time to be a discrete quantity then it is natural to try to define a Wigner function in this setting. An early attempt was made by Chan [13] and it coincides with the modified Wigner function defined by Bizarro. A review of several approaches to Time-Frequency analysis with discrete time applied to Fusion Plasmas is given in [14].

1.4 Objectives and Deliverables

The main objective of this thesis is to study the Quantum Pendulum in the Wigner function representation. For that an associated solvable model will also be studied. The association between the stationary pure states of the Quantum Pendulum and Mathieu functions of even index will also be explored. In order to study pure states the Quantum Pendulum will also be studied in the Density Operator representation. Additionally, a simplified way of obtaining the evolution equations in the Wigner function representation will be presented.

The main deliverables will be explicit solutions to the stationarity equations, both in the Wigner function representation and Density Operator representation. Since these do not necessarily represent pure states, a basis of the space of stationary solutions should be presented. Finally, the translation of these solutions into solutions of the Helmholtz equation in two dimensions is to be developed.

1.5 Thesis Outline

In chapter 2 we will start by making some general remarks about the Quantum Mechanics of angular variables and their link to Tight-Binding models. A few observations about perturbation theory in this setting will also be made. Next, I will review the most important facts about Mathieu functions that will be of interest to us. Following that, the brief review of the Wigner function presented in this Introduction will be complemented and the integral form of the Moyal product will be presented. Then it is time to present two new simplified ways of obtaining the evolution equations. Chapter 2 ends with some remarks about pure states and integral kernels of integral operators plus their connection to the Helmholtz equation in two dimensions.

Chapter 3 is the main chapter of this thesis. Five different families of solutions to the stationarity equation in the Wigner function representation will be given. Several ways to achieve them will be presented and compared. Finally, the Wigner transforms of solutions to the Helmholtz 2d equation in modified elliptic coordinates will be computed and compared to the solutions previously obtained.

Chapter 4 is about the Density Operator representation. We will start by giving explicit formulas for the matrix elements of stationary operators in the angular momentum basis. Following that, the connection to solutions of the Helmholtz equation in two dimensions will be explored. We end chapter 4 with a discussion of stategies to try to obtain closed form expressions for the even Mathieu functions of even index.

For the reader's convenience an appendix with generalities about (Generalized) Hypergeometric Functions is available at the end of the thesis. In this Appendix A the reader will find a discussion of notation, the basic facts about the Mellin transform and a collection of the Bessel function identities that will be used in the main text. The final appendix involves some computations that do not properly belong to the main text and contains a formula about Chebyshev polynomials that is likely new.

Chapter 2

Quantum Mechanics Background

2.1 Quantum Mechanics of Angular Variables

The purpose of this section is to introduce the main Hamiltonians that will be studied in this Thesis and to make some general remarks about perturbation theory in the Schrödinger representation.

2.1.1 Angular momentum and Tight-Binding

We start by observing that unlike with the usual cartesian coordinates x, p for position and momentum, when using cylindrincal coordinates θ, l in the Scrödinger representation, an immediate quantization occurs: the angular momentum l comes in discrete units of $\hbar$, that is, $l = \hbar m$, with m an integer. This is obvious from Fourier analysis, the Fourier transform of a periodic function is given by a Fourier series. In the setting of Abstract Harmonic Analysis one would say that the dual group of S^1 is $\mathbb{Z}$ and the dual group of $\mathbb{Z}$ is S^1. This introduces an important practical difference between the coordinate and momentum representations, while in the former one works with differential equations, in the latter one deals with difference equations.

It is interesting to observe that what constitutes coordinate and what constitutes momentum depends on the setting. For example, in Tight-Binding models the discrete variable n is a position variable and the crystal momentum k is the continuous periodic variable. Since Tight-Binding models are approximations to continuous models, in this work we will adopt the more fundamental convention that the angular variable is the coordinate variable and the discrete variable is the angular momentum variable. Another useful convention we will adopt from now on is that we always work with the angular-momentum basis, that is, the vectors $|m\rangle$ are the functions $\frac{1}{\sqrt{2\pi}}e^{im\theta}$, with m an integer, and they satisfy $\hat{l}|m\rangle = \hbar m|m\rangle$, where the angular-momentum operator $\hat{l}$ is given by $\hat{l} = -i\hbar\partial/\partial\theta$. In the rare occasions in which the angular coordinate basis $|\theta\rangle$ will appear it will be obvious from the context that the vectors are the periodic delta functions

$$\check{\delta}(\theta' - \theta) = \sum_{n=-\infty}^{\infty} \delta(\theta' - \theta - 2\pi n) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} e^{in(\theta' - \theta)}. \tag{2.1}$$

The two main Hamiltonians we will be working with are the *Simplified Hindered Rotator* (SHR)

$$\hat{H}_{SHR} = \omega\hat{l} - \lambda\cos(\hat{\theta}), \tag{2.2}$$

where the frequency ω and the energy λ are parameters, and the *Quantum Pendulum* (QP)

$$\hat{H}_{QP} = \frac{\hat{l}^2}{2I} - \lambda\cos(\hat{\theta}), \tag{2.3}$$

where again the moment of inertia I and the energy λ are parameters. Notice that in the classical case λ would be the famous mgl. The terminology "Simplified Hindered Rotator" comes from the *Hindered Rotator*

$$\hat{H}_{HR} = \omega\big|\hat{l}\big| - \lambda\cos(\hat{\theta}), \tag{2.4}$$

introduced by Berry in [7] and extensively studied by Bizarro in [2]. The SHR model is not physically realistic since its spectrum is not bounded below, but it is a solvable model and was used implicitly in [2] as an approximation.

Writing the time-independent Schrödinger equation $\hat{H}|\psi\rangle = E|\psi\rangle$ in Fourier space, we have for the SHR model

$$\hbar\omega n\tilde{\psi}(n) - 2\lambda\big(\tilde{\psi}(n+1) + \tilde{\psi}(n-1)\big) = E\tilde{\psi}(n), \tag{2.5}$$

and

$$\frac{\hbar^2}{2I}n^2\tilde{\psi}(n) - 2\lambda\big(\tilde{\psi}(n+1) + \tilde{\psi}(n-1)\big) = E\tilde{\psi}(n), \tag{2.6}$$

for the QP model. Defining the adimensional parameters $\bar{\lambda} = -\frac{\hbar\omega}{2\lambda}$ and $\bar{\lambda} = -\frac{\hbar^2}{4\lambda I}$ for the SHR and QP models, respectively, the above equations can be written as

$$\bar{\lambda}n\tilde{\psi}(n) + \tilde{\psi}(n+1) + \tilde{\psi}(n-1) = \bar{E}\tilde{\psi}(n), \tag{2.7}$$

and

$$\bar{\lambda}n^2\tilde{\psi}(n) + \tilde{\psi}(n+1) + \tilde{\psi}(n-1) = \bar{E}\tilde{\psi}(n). \tag{2.8}$$

These equations have the form of three-term recurrences as the well-known *Almost Mathieu operator* or *Aubry-André* model

$$\bar{\lambda}\cos(2\pi\tau n + \omega_0)\tilde{\psi}(n) + \tilde{\psi}(n+1) + \tilde{\psi}(n-1) = \bar{E}\tilde{\psi}(n), \tag{2.9}$$

where τ, ω_0 are additional parameters and τ is assumed to be irrational. Yet another variation is the *Maryland* model

$$\bar{\lambda}\tan(2\pi\tau n + \omega_0)\tilde{\psi}(n) + \tilde{\psi}(n+1) + \tilde{\psi}(n-1) = \bar{E}\tilde{\psi}(n). \tag{2.10}$$

Given any $\bar{E}, \bar{\lambda}$ and initial conditions $\tilde{\psi}(0), \tilde{\psi}(1)$ there is a unique solution $\tilde{\psi}(n)$ defined for all integer n for any of these equations. But, and this is the main point, for a fixed $\bar{\lambda}$ there are, if any, at most countably many eigenvalues $\bar{E}$ that give rise to a solution $\tilde{\psi}(n)$ that is normalizable, that is,

$$\sum_{n=-\infty}^{\infty} |\tilde{\psi}(n)|^2 < \infty. \tag{2.11}$$

In fact, for a fixed $\bar{\lambda}$ even the set of $\bar{E}$ for which a solution exists that only grows polinomially is usually restricted (those values are sometimes called *pseudo-eigenvalues* or *generalized eigenvalues*, although the latter terminology has a different meaning in Linear Algebra).

The existence of eigenvalues usually depends on the diophantine properties of τ, but for the Simplified Hindered Rotator and the Quantum Pendulum, a discrete set of eigenvalues exists for any value of $\bar{\lambda}$ and the corresponding eigenfunctions form a basis of the Hilbert space.

2.1.2 Perturbation Theory

The number of models in Quantum Mechanics that are exactly solvable is not staggering. The ones one learns about in a first course in Quantum Mechanics are the Particle in a Box, the Harmonic Oscillator and the Hydrogen Atom. These have the property that the spectrum of the Hamiltonian is a simple algebraic function of the coupling constant. In the first case, $E = (\hbar\pi n)^2/2ma^2$, in the second $E = \hbar\omega(n + 1/2)$ and in the third $E = -\mu(Z\alpha c)^2/2n^2$. If the spectrum varies in a non-trivial way with the coupling constant an exact form for the solutions is much more difficult to achieve. As will be seen in the next section the SHR model is exactly solvable and its spectrum does not vary with the coupling constant, only the eigenfunctions do.

Perturbation theory is a systematic method to obtain solutions as a power series expansion on an appropriate coupling constant. In the setting of the previous section, perturbation theory is especially simple. No integrals are to be computed. A simple recurrence is enough to obtain the terms up to any power of the coupling constant. To see this write κ for $1/\bar{\lambda}$. All the three-term equations in the previous section have the form:

$$f(n)\tilde{\psi}(n) + \kappa\tilde{\psi}(n+1) + \kappa\tilde{\psi}(n-1) = E'\tilde{\psi}(n). \tag{2.12}$$

Now, expanding the Fourier coefficients and the eigenvalue as powers of κ:

$$\tilde{\psi}(n) = \sum_{j=0}^{\infty} b(n,j)\kappa^j, \qquad E' = \sum_{j=0}^{\infty} g_j\kappa^j, \tag{2.13}$$

one must have

$$f(n)b(n,j) + b(n+1,j-1) + b(n-1,j-1) = \sum_{l=0}^{j} g_l b(n,j-l), \tag{2.14}$$

for all $j \geq 0$, where we make the convention $b(n,-j) = 0$ for positive j.

When $\kappa = 0$ in (2.12), the eigenfunctions are given by $\tilde{\psi}(n) = \delta_{n,m}$ and the eigenvalues by $E' = f(m)$, where m is an integer. That is, the Hamiltonian is of the form $\hat{H} = f(\hat{l})$ and the eigenfunctions are the eigenfunctions $|m\rangle$ of the angular momentum operator $\hat{l}$. From the point of view of perturbation theory, the coefficients g_0 are always of the form $f(m)$ and the coefficients $b(n,0)$ always of the form $\delta_{n,m}$ times a normalization constant.

With this information we can start to compute all the coefficients $b(n,j)$ and g_j for a fixed unperturbed m. Doing this one will quickly come to the following conclusions. First, that for a fixed integer n, the first Taylor coefficient $b(n,j)$ that is different from zero is $j = |n-m|$. So, $b(n,j) = 0$ for $j < |n-m|$. Equation (2.14) imposes a certain speed of propagation of the effects of the coefficients. Second, the coefficients $b(m,j)$ for $j > 0$ are not determined. This is a manifestation of the fact that the time-independent Schrödinger equation is a linear equation, hence one can multiply a wave function $|\psi\rangle$ solution by any constant and still have a solution. From the point of view of the three-term equation (2.12) this means that the Fourier coefficient $\tilde{\psi}(m)$ is not determined as a function of κ, only its value at $\kappa = 0$ is. So we can choose the coefficients $b(m,j)$ as we please. A popular choice is $b(m,j) = 0$ for $j > 0$. This speeds up the numerical computations, but may not be the best from an analytical perspective. For example, if $\tilde{\psi}(m)$ has a zero as a function of κ then the power series for the other coefficients will have a finite radius of convergence.

Two more patterns can be observed. The first is that for a given integer n the value of the first Taylor coefficient different from zero $b(n,|n-m|)$ does not depend on the normalization of the wave function for $\kappa \neq 0$. The second is that if we choose $\tilde{\psi}(m)$ to be an even function of κ, that is, $b(m,j) = 0$ for all odd j, then $\tilde{\psi}(m+1)$ and $\tilde{\psi}(m-1)$ will be odd functions of κ, $\tilde{\psi}(m+2)$ and $\tilde{\psi}(m-2)$ will be even functions of κ, $\tilde{\psi}(m+3)$ and $\tilde{\psi}(m-3)$ will be odd functions of κ, and so on, the parity of the Fourier coefficients as functions of κ will be alternating.

2.1.3 The Simplified Hindered Rotator

In eq. (2.2) we defined the Simplified Hindered Rotator $\hat{H}_{SHR} = \omega\hat{l} - \lambda\cos(\hat{\theta})$. In this section we will see that this is a solvable model. First we will look at the time-independent Schrödinger equation in coordinate space and then in angular momentum space.

Differential equation

In the case of the SHR, the eigenfunctions are actually very easy to obtain because the time-independent Schrödinger equation is the first-order linear differential equation

$$-i\hbar\omega\frac{d\psi}{d\theta}(\theta) - \lambda\cos(\theta)\psi(\theta) = E\psi(\theta), \tag{2.15}$$

whose solution is obtained straightforwardly by separation of variables:

$$\int\frac{d\psi}{\psi} = \frac{i}{\hbar\omega}\int[E + \lambda\cos(\theta)]d\theta + C, \tag{2.16}$$

with C some arbitrary constant. Therefore,

$$\psi(\theta) = \frac{1}{\sqrt{2\pi}}e^{i\frac{E}{\hbar\omega}\theta}e^{i\frac{\lambda}{\hbar\omega}\sin(\theta)} \tag{2.17}$$

and we see that $E/\hbar\omega$ must be an integer for the solution to have period 2π. Notice that the energies $E = \hbar\omega d$ do not depend on the potential-energy strength λ, only the eigenfunctions do.

Difference equations

We can now note that the second exponential factor in (2.17) is the generating function for Bessel functions (A.26), whence, defining $d = E/\hbar\omega \in \mathbb{Z}$ and $c = -\lambda/2\hbar\omega$, we can write the eigenfunctions as

$$\psi_d(\theta) = \frac{1}{\sqrt{2\pi}} e^{id\theta} \sum_{r=-\infty}^{\infty} J_r\left(\frac{\lambda}{\hbar\omega}\right) e^{ir\theta} = \frac{1}{\sqrt{2\pi}} \sum_{r=-\infty}^{\infty} J_{r-d}\left(-2c\right) e^{ir\theta}. \tag{2.18}$$

This gives us an explicit form for the Fourier coefficients of the solutions of the time-independent Schrödinger equation. One could also have obtained this explicit form from the three-term equation (2.12) as was done by Bizarro in [2]. The equation in this case reads

$$n\tilde{\psi}(n) + c\tilde{\psi}(n+1) + c\tilde{\psi}(n-1) = E'\tilde{\psi}(n) \tag{2.19}$$

and noticing that Bessel functions satisfy the relation (A.23)

$$2nJ_n(z) - zJ_{n-1} - zJ_{n+1}(z) = 0 \tag{2.20}$$

we get

$$\tilde{\psi}(n) = NJ_{n-d}(-2c) \quad \text{and} \quad E = \hbar\omega d \tag{2.21}$$

where N a normalization constant and d is an integer. One then sees that $N = 1/\sqrt{2\pi}$ in the case at hand.

If we had started from the perturbation theory equation

$$nb(n,j) + b(n+1, j-1) + b(n-1, j-1) = \sum_{l=0}^{j} g_l b(n, j-l), \tag{2.22}$$

we would come to notice that all the g_j with $j > 0$ that we computed were zero. Conjecturing then that indeed $g_j = 0$ for all $j > 0$, we would try to solve the equation

$$(n-m)b(n,j) + b(n+1, j-1) + b(n-1, j-1) = 0. \tag{2.23}$$

Considering the power series form of Bessel functions (A.22)

$$J_n(z) = \left(\frac{z}{2}\right)^n \sum_{k=0}^{\infty} \frac{(-1)^k z^{2k}}{4^k k!(k+n)!} \tag{2.24}$$

one can verify that

$$b(n,j) = \frac{(-1)^{\frac{j-n+m}{2}}}{\left(\frac{j-n+m}{2}\right)!\left(\frac{j+n-m}{2}\right)!} \tag{2.25}$$

where j has the same parity as $n-m$, and $b(n,j)=0$ otherwise, indeed solves eq. (2.23). It should be noted that the normalization $b(m,2j)=(-1)^j/j!j!$ is not something we could have easily guessed to give a closed form without extensive analysis of the partial difference equation.

In the more symmetric case $m=0$ we will see in section 3.2.1 that there is a more global way to try to solve the partial difference equation (look at eq. (3.20) there, it is closely associated to eq. (2.23)).

2.2 Mathieu Functions and Perturbation Theory

The Hamiltonian of the Quantum Pendulum was defined in eq. (2.3) by $\hat{H}_{QP}=\frac{\hat{l}^2}{2I}-\lambda\cos(\hat{\theta})$. In this section we will review the connection between the eigenfunctions of this Hamiltonian and the Mathieu functions of even order.

2.2.1 The Quantum Pendulum and Mathieu functions

In the QP case, the eigenfunctions satisfy the equation

$$-\frac{\hbar^2}{2I}\frac{d^2\psi}{d\theta^2}(\theta)-\lambda\cos(\theta)\psi(\theta)=E\psi(\theta), \tag{2.26}$$

which is a particular case of the Mathieu equation whose standard form reads [15–20]:

$$\frac{d^2f}{dz^2}(z)+[a-2q\cos(2z)]f(z)=0. \tag{2.27}$$

For every q there is a discrete set of values for a (the so-called *characteristic values*) for which this equation has periodic solutions, either with period π or with period 2π. The former are called the *Mathieu functions* of even order, usually denoted by $ce_{2n}(z,q)$ and $se_{2n+2}(z,q)$, and are the solutions that interest us, since we are going to look for solutions of period 2π (in θ) after making the change of variables $\theta=2z$ and $\psi(\theta)=f(\theta/2)$. The Mathieu equation (2.27) then becomes

$$4\frac{d^2\psi}{d\theta^2}(\theta)+[a-2q\cos(\theta)]\psi(\theta)=0 \tag{2.28}$$

and, comparing with (2.26), we see that $E=\hbar^2a/8I$ and $q=-4\lambda I/\hbar^2=4c$, the QP problem having been thus reduced to the study of the Mathieu functions of even order. Unfortunately, for over 150 years of research no closed forms have yet been reached for the Mathieu functions of even (or odd) order. One of the main themes of this thesis is to argue that the study of the Wigner transform of stationary solutions of the Quantum Pendulum may give us such closed forms. In order to do that we need to learn a bit more about Mathieu functions.

The functions $ce_{2n}(z,q)$ are even functions of z and the functions $se_{2n+2}(z,q)$ are odd functions of z. Hence the notation, the “c” in ce should remind us of cosine and the “s” in se of sine. When $q=0$, $ce_{2n}(z,0)=\cos(2nz)$ and $se_{2n+2}(z,0)=\sin((2n+2)z)$. The Fourier coefficients of the Mathieu functions are named *Mathieu coefficients*, and the usual notation for the cosine-Fourier coefficients of $ce_{2n}(z,q)$

and the sine-Fourier coefficients of $se_{2n+2}(z,q)$ is $A_{2r}^{(2n)}(q)$ and $B_{2r+2}^{(2n+2)}(q)$, respectively. That is,

$$ce_{2n}(z,q) = \sum_{r=0}^{\infty} A_{2r}^{(2n)}(q)\cos(2rz), \tag{2.29}$$

and

$$se_{2n+2}(z,q) = \sum_{r=0}^{\infty} B_{2r+2}^{(2n+2)}(q)\sin((2r+2)z) \tag{2.30}$$

The Mathieu coefficients are analytic functions of the parameter q but, as already said, no closed forms are known for their expressions. The eigenvalues associated to the Mathieu functions are called *characteristic numbers* and are denoted by $a_{2n}(q)$ and $b_{2n+2}(q)$ for the even and odd Mathieu functions, respectively. From the three-term relations

$$\begin{aligned} aA_0 - qA_2 &= 0 \\ (a-4)A_2 - q(A_4 + 2A_0) &= 0 \\ (a-4r^2)A_{2r} - q(A_{2r+2} + A_{2r-2}) &= 0, \text{ for } r \geq 2 \end{aligned} \tag{2.31}$$

and

$$\begin{aligned} (a-4)B_2 - qB_4 &= 0 \\ (a-4r^2)B_{2r} - q(B_{2r+2} + B_{2r-2}) &= 0, \text{ for } r \geq 2, \end{aligned} \tag{2.32}$$

one can see that the characteristic numbers are given by ratios of Mathieu coefficients:

$$a_{2n}(q) = \frac{qA_2^{(2n)}(q)}{A_0^{(2n)}(q)} \quad \text{and} \quad b_{2n+2}(q) = 4 + \frac{qB_4^{(2n+2)}(q)}{B_2^{(2n+2)}(q)}. \tag{2.33}$$

So, having a closed form for Mathieu coefficients gives us immediately a closed form for the characteristic numbers.

There is really no standard normalization for Mathieu functions. The original normalization used by Mathieu [1] is good for perturbation theory, but differs from the Hilbert space normalization. Frequently, a middle ground is achieved by putting $\langle\psi|\psi\rangle$ equal to π or 2π. It is the working hypothesis of this thesis that there might be a normalization depending on q for which the Mathieu coefficients can be written in a closed form. If this is the case then the passage to more standard normalizations such as the Hilbert space normalization is straightforward.

To finish this section notice the awkward factor 2 for A_0 in the middle equation of (2.31). This comes from not working with complex Fourier coefficients. In the following we will work only with complex Fourier coefficients, but will have to, sometimes, make the connection to cosine-Fourier and sine-Fourier coefficients. Working with complex Fourier coefficients transforms the multiple relations in (2.31) and (2.32) into a single relation. Also recall that our variable θ is equal to $2z$. This means that our eigenfunctions will be given by $ce_{2n}(\theta/2)$ and $se_{2n+2}(\theta/2)$ and, consequently, that we will have to divide the index of the Fourier coefficients by 2. That is, $\langle r|\psi\rangle$ refers to the real or imaginary parts of $A_{2|r|}$ and $B_{2|r|}$ times a normalization constant. This takes care of the awkwardness of the factor 2.

2.2.2 Perturbation theory for Mathieu functions

The traditional path [16] to obtain information about the Mathieu coefficients is equivalent to doing time-independent perturbation theory as in section 2.1.2. For our purposes, we will only quote some of the results in the literature. The first non-zero Taylor coefficients of Mathieu coefficients as functions of the parameter q are known [16–18] and read:

$$A_{2n+2r}^{(2n)}(q) \simeq (-1)^r \frac{(2n)!}{r!(2n+r)!} \left(\frac{q}{4}\right)^r \simeq B_{2n+2r}^{(2n)}(q) \tag{2.34}$$

$$A_{2n-2r}^{(2n)}(q) \simeq \frac{(2n-r-1)!}{r!(2n-1)!} \left(\frac{q}{4}\right)^r \simeq B_{2n-2r}^{(2n)}(q) \tag{2.35}$$

for $n > 0$ and $r \geq 0$,

$$A_{2r}^{(0)}(q) \simeq (-1)^r \frac{2}{r!r!} \left(\frac{q}{4}\right)^r \tag{2.36}$$

for $r > 0$, and we always have

$$A_{2n}^{(2n)}(q) \simeq 1 \simeq B_{2n}^{(2n)}. \tag{2.37}$$

Looking at these formulas we see that it is natural to define the coupling constant as $c = q/4 = -\lambda I/\hbar^2$.

Our effort to obtain closed forms for Mathieu functions will lead us in chapter 4 to look at products of Mathieu coefficients. From the formulas above we have

$$\frac{1}{\sqrt{2\pi}} \langle r|ce_{2n}\rangle = \begin{cases} \frac{1}{2} A_{|2r|}^{(2n)} & \text{if } r \neq 0 \\ A_0^{(2n)} & \text{if } r = 0, \end{cases} \tag{2.38}$$

so that, for instance, if $r, s \geq n > 0$, we get from (2.34) (with r replaced with $r - n$)

$$\frac{1}{2\pi} \langle r|ce_{2n}\rangle\langle ce_{2n}|s\rangle \simeq \frac{1}{4}(-1)^{r+s-2n} \frac{(2n)!(2n)!}{(r-n)!(r+n)!(s-n)!(s+n)!} c^{r+s-2n}. \tag{2.39}$$

If $n = 0$ we have a quite simple formula for $r, s \geq 0$,

$$\frac{1}{2\pi} \langle r|ce_0\rangle\langle ce_0|s\rangle \simeq (-1)^{r+s} \frac{1}{r!r!s!s!} c^{r+s}. \tag{2.40}$$

These formulas will be referred to in chapter 4.

2.3 The Wigner-Chan-Bizarro function

As described in section 1.2 of the Introduction, Bizarro in his Ph.D. thesis [2] provided a new definition of the Wigner function for angular variables. The reader should nevertheless be aware that that was not how he saw it. For him the new definition was simply an auxiliary definition and not meant to substitute the one given by Berry and Mukunda [7, 8]. I disagree with that view and think that the benefits of the new definition are so many that it should be considered at least in an equal footing with the older definition.

In this section we review the relevant formulas from the Introduction that will be used in the following, plus two extra formulas. Additionally, we give some examples of Wigner transforms and conclude with the integral form of the Moyal product.

We start by recalling the definition of the modified Wigner function

$$w(\theta, m) = \frac{1}{2\pi} \sum_{\substack{m' \text{ same} \\ \text{parity as } m}} e^{i\theta m'} \langle \tfrac{m+m'}{2} | \psi \rangle \langle \psi | \tfrac{m-m'}{2} \rangle. \tag{2.41}$$

I think it is not inappropriate to designate such an object by the *Wigner-Chan-Bizarro* function. Next we recall the generalization of this modified Wigner transform to operators:

$$a(\theta, m) = \frac{1}{2\pi} \sum_{\substack{m' \text{ same} \\ \text{parity as } m}} e^{i\theta m'} \langle \tfrac{m+m'}{2} | \hat{A} | \tfrac{m-m'}{2} \rangle. \tag{2.42}$$

For future reference, we also give two additional useful formulas. The first is the formula for the modified Wigner transform of a general operator $\hat{A}$ computed in the angular basis

$$a(\theta, m) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta' e^{-im\theta'} \langle \theta + \theta' | \hat{A} | \theta - \theta' \rangle; \tag{2.43}$$

the second is the relation between the classical Wigner transform of a periodic function, with period L, and the modified Wigner transform [21]

$$W(x, p) = \tfrac{2\pi}{\hbar L} \sum_{m=-\infty}^{\infty} \delta\left(\tfrac{p}{\hbar} - \tfrac{\pi m}{L}\right) w\left(\tfrac{2\pi x}{L}, m\right), \tag{2.44}$$

where it is supposed that the periodic function is normalized in an interval of period L. Notice that the wave number $p/\hbar$ is a multiple of π/L and not of $2\pi/L$, this is a manifestation of the doubling of points characteristic of Wigner functions.

In the author's view equations (2.42), (2.43) and (2.44) provide the strongest argument in favour of viewing the modified Wigner function as the true Wigner function for angular variables. The first two equations by their symmetry. The original Wigner function of Berry and Mukunda when written in the angular momentum basis [2] is incredibly complicated, it involves two sums and the second sum is actually a double sum, while the modified one is entirely symmetric in the roles of θ and m. The third equation also provides a very strong argument in favour of considering the new definition as the correct one since it is simply what one obtains from the original definition of Wigner when applied to periodic functions.

2.3.1 Examples

In this section we give some examples of modified Wigner transforms.

The first two examples appeared in [2] and can easily be computed using formula (2.42). The first example is given by the Wigner transform of an Hamiltonian of the form $\hat{H} = f(\hat{l})$ where $\hat{l}$ is the angular momentum operator and $f(l)$ is an arbitrary function. In this case

$$h(\theta, m) = \begin{cases} \frac{1}{2\pi} f\left(\frac{\hbar m}{2}\right) & \text{if } m \text{ even} \\ 0 & \text{if } m \text{ odd.} \end{cases} \tag{2.45}$$

In this thesis two such cases occur with $f_1(l) = \omega l$ and $f_2(l) = l^2/2I$. The second example is given by the Wigner transform of an Hamiltonian of the form $\hat{H} = -\lambda \cos(\theta)$. Here we get

$$h(\theta, m) = \begin{cases} 0 & \text{if } m \text{ even} \\ -\frac{\lambda}{2\pi} \cos(\theta) & \text{if } m \text{ odd.} \end{cases} \tag{2.46}$$

Since the Wigner transform is linear, the Wigner transform of the Hamiltonian of the Quantum Pendulum becomes

$$h_{QP}(\theta, m) = \begin{cases} \frac{\hbar^2 m^2}{8\pi I} & \text{if } m \text{ even} \\ -\frac{\lambda}{2\pi} \cos(\theta) & \text{if } m \text{ odd.} \end{cases} \tag{2.47}$$

The next example is the Wigner transform of the eigenfunctions of the Simplified Hindered Rotator. There are two ways to compute this, but in their essence both use the generating function for Bessel functions (A.26). In the first way one notices that (2.17) is the expression for a Frequency-Modulated (FM) signal if we substitute θ by $2\pi t/T$. The Wigner transform of a FM signal is known [22] (see also [4]; in (8.56) there, put $\beta = 0$, $m = \lambda/\hbar\omega = -2c$, $\omega_m = 2\pi/L$, $\omega_0 = 2\pi d/L$, multiply everything by $(\pi/\alpha L^2)^{\frac{1}{4}}$ and make α tend to zero):

$$W\left(\tfrac{L\theta}{2\pi}, p\right) = \tfrac{1}{L\hbar} \sum_{n=-\infty}^{\infty} \delta\left(\tfrac{p}{\hbar} - \tfrac{n\pi}{L} - \tfrac{2\pi d}{L}\right) J_n[-4c\cos(\theta)] \tag{2.48}$$

hence, by (2.44)

$$w(\theta, m) = \frac{1}{2\pi} J_{m-2d}[-4c\cos(\theta)]. \tag{2.49}$$

In the second way, which is actually simpler, one uses eq. (2.41) with the Fourier coefficients in (2.18) and then use Graf's formula (A.29) for the Fourier coefficients of a Bessel function composed with a cosine in a way similar to what Bizarro did in section V.B of his [2].

2.3.2 The Moyal product in integral form

The differential form of the Moyal bracket is exceedingly complicated. By contrast, the integral form is actually quite simple. If $a(\theta, m)$ and $b(\theta, m)$ are the Wigner transforms of operators $\hat{A}$ and $\hat{B}$, then their Moyal product is given by

$$a \bigstar b(\theta, m) = \frac{1}{2\pi} \int_0^{2\pi} d\theta' \int_0^{2\pi} d\theta'' \sum_{\substack{m', m'': \\ m'+m'' \text{ same} \\ \text{parity as } m}} a(\theta + \theta', m + m') b(\theta + \theta'', m + m'') e^{i(\theta' m'' - \theta'' m')}. \tag{2.50}$$

This expression can be verified using (2.42). We have then

$$a\bigstar b(\theta,m)=\frac{1}{(2\pi)^3}\int_0^{2\pi}d\theta'\int_0^{2\pi}d\theta''\sum_{\substack{m',m'':\\ m'+m''\text{ same}\\ \text{parity as }m}}\sum_{\substack{n'\text{ same}\\ \text{parity as }m+m'}}\sum_{\substack{n''\text{ same}\\ \text{parity as }m+m''}}e^{in'(\theta+\theta')}$$
$$\cdot\langle\tfrac{m+m'+n'}{2}|\hat{A}|\tfrac{m+m'-n'}{2}\rangle e^{in''(\theta+\theta'')}\langle\tfrac{m+m''+n''}{2}|\hat{B}|\tfrac{m+m''-n''}{2}\rangle e^{i(\theta'm''-\theta''m')}. \tag{2.51}$$

We can rewrite the exponentials in the form

$$e^{i(n'+n'')\theta}e^{i(n'+m'')\theta'}e^{i(n''-m')\theta''} \tag{2.52}$$

and integrate in θ' and θ''. Only the terms with $n'=-m''$ and $n''=m'$ survive. Hence

$$a\bigstar b(\theta,m)=\frac{1}{2\pi}\sum_{\substack{n',n'':\\ n'+n''\text{ same}\\ \text{parity as }m}}e^{i(n'+n'')\theta}\langle\tfrac{m+n''+n'}{2}|\hat{A}|\tfrac{m+n''-n'}{2}\rangle\langle\tfrac{m-n'+n''}{2}|\hat{B}|\tfrac{m-n'-n''}{2}\rangle. \tag{2.53}$$

Defining new variables $n=n'+n''$ and $r=(m-n'+n'')/2$ this can be written as

$$a\bigstar b(\theta,m)=\frac{1}{2\pi}\sum_{\substack{n\text{ same}\\ \text{parity as }m}}\sum_{r=-\infty}^{\infty}e^{in\theta}\langle\tfrac{m+n}{2}|\hat{A}|r\rangle\langle r|\hat{B}|\tfrac{m-n}{2}\rangle=\frac{1}{2\pi}\sum_{\substack{n\text{ same}\\ \text{parity as }m}}e^{in\theta}\langle\tfrac{m+n}{2}|\hat{A}\hat{B}|\tfrac{m-n}{2}\rangle, \tag{2.54}$$

which is what we wanted to verify. The Moyal bracket is then $[a,b]_\star=a\bigstar b-b\bigstar a$. This can be written succintly as

$$[a,b]_\star(\theta,m)=\frac{1}{2\pi}\int_0^{2\pi}d\theta'\int_0^{2\pi}d\theta''\sum_{\substack{m',m'':\\ m'+m''\text{ same}\\ \text{parity as }m}}a(\theta+\theta',m+m')b(\theta+\theta'',m+m'')2i\sin(\theta'm''-\theta''m'), \tag{2.55}$$

but in practice it is best to compute the terms $a\bigstar b$ and $b\bigstar a$ separately.

2.4 The evolution equation

2.4.1 Evolution of the density operator

The equation giving the evolution of the density operator is

$$i\hbar\frac{d}{dt}\hat{\rho}(t)=[\hat{H},\hat{\rho}(t)], \tag{2.56}$$

which, in terms of the matrix elements $\hat{A}_{r,s}=\langle r|\hat{A}|s\rangle$, reads

$$i\hbar\frac{d\hat{\rho}_{r,s}}{dt}=[\hat{H},\hat{\rho}]_{r,s}. \tag{2.57}$$

Computation of the right-hand side of (2.57) is very simple: if, say, $\hat{H}$ is just a function of the angular momentum, meaning $\hat{H} = f(\hat{l})$, then

$$\begin{aligned}[f(\hat{l}), \hat{\rho}]_{r,s} &= \langle r|[f(\hat{l}), \hat{\rho}]|s\rangle = \langle r|f(\hat{l})\hat{\rho} - \hat{\rho} f(\hat{l})|s\rangle = (f(\hbar r) - f(\hbar s))\langle r|\hat{\rho}|s\rangle \\ &= (f(\hbar r) - f(\hbar s))\hat{\rho}_{r,s}, \end{aligned} \tag{2.58}$$

whereas, if $\hat{H}$ acts by multiplication, and noticing that $e^{in\hat{\theta}}|m\rangle = |m+n\rangle$, we have, for instance with $\hat{H} = \cos(\hat{\theta})$,

$$\begin{aligned}[\cos(\hat{\theta}), \hat{\rho}]_{r,s} &= \langle r|\tfrac{e^{i\hat{\theta}}+e^{-i\hat{\theta}}}{2}\hat{\rho} - \hat{\rho}\tfrac{e^{i\hat{\theta}}+e^{-i\hat{\theta}}}{2}|s\rangle \\ &= \tfrac{1}{2}\big(\langle r-1|\hat{\rho}|s\rangle + \langle r+1|\hat{\rho}|s\rangle - \langle r|\hat{\rho}|s+1\rangle - \langle r|\hat{\rho}|s-1\rangle\big) \\ &= \tfrac{1}{2}\big(\hat{\rho}_{r-1,s} + \hat{\rho}_{r+1,s} - \hat{\rho}_{r,s+1} - \hat{\rho}_{r,s-1}\big), \end{aligned} \tag{2.59}$$

which now has the form of a difference equation.

If $\hat{H}$ is the sum of an angular-momentum part plus an angle-dependent potential part, then we just use the linearity of $[.,\hat{\rho}]$. As examples (with ω, λ, and I positive constants), take the SHR and QP Hamiltonians, respectively, $\hat{H} = \omega\hat{l} - \lambda\cos(\hat{\theta})$ and $\hat{H} = \hat{l}^2/2I - \lambda\cos(\hat{\theta})$, in which cases (2.57) becomes

$$\boxed{i\hbar\frac{d\hat{\rho}_{r,s}}{dt} = \hbar\omega(r-s)\hat{\rho}_{r,s} - \frac{\lambda}{2}\big(\hat{\rho}_{r-1,s} + \hat{\rho}_{r+1,s} - \hat{\rho}_{r,s+1} - \hat{\rho}_{r,s-1}\big)} \tag{2.60}$$

and

$$\boxed{i\hbar\frac{d\hat{\rho}_{r,s}}{dt} = \frac{\hbar^2}{2I}(r^2 - s^2)\hat{\rho}_{r,s} - \frac{\lambda}{2}\big(\hat{\rho}_{r-1,s} + \hat{\rho}_{r+1,s} - \hat{\rho}_{r,s+1} - \hat{\rho}_{r,s-1}\big).} \tag{2.61}$$

2.4.2 Evolution of the modified Wigner transform

We now allow our Wigner functions to evolve over time, that is, $w = w(\theta, m, t)$, the analogue of the evolution equation being

$$i\hbar\frac{\partial w}{\partial t} = [h, w]_\star. \tag{2.62}$$

Bizarro [2] obtained the final evolution equation in two steps: first, the phase-space function $h(\theta, m)$ was calculated and, second, the Moyal parenthesis $[h, w]_\star$ was computed. In this subsection it is shown that it is easier to start from the equation for the density operator and subsequently translate it into an equation for the time-evolution of the Fourier coefficients of $w(\theta, m, t)$, which is then translated into the final equation for $\partial w/\partial t$.

Evolution of the Fourier coefficients

If we expand the modified Wigner transform into a Fourier series

$$w(\theta, m, t) = \frac{1}{2\pi} \sum_{\substack{n \text{ same} \\ \text{parity as } m}} a_{m,n}(t) e^{in\theta}, \tag{2.63}$$

it is evident from (2.41) that the Fourier coefficients $a_{m,n}$ for m and n of the same parity are given by

$$a_{m,n}(t) = \langle \tfrac{m+n}{2} | \hat{\rho}(t) | \tfrac{m-n}{2} \rangle. \tag{2.64}$$

If we change variables according to $r = (m+n)/2$ and $s = (m-n)/2$, which leads to $m = r+s$ and $n = r-s$, hence to

$$a_{r+s,r-s}(t) = \langle r | \hat{\rho}(t) | s \rangle, \tag{2.65}$$

then the difference-differential equations (2.60) and (2.61) become equations for the Fourier coefficients.

For the SHR model we have

$$i\hbar \frac{da_{r+s,r-s}}{dt} = \hbar\omega(r-s) a_{r+s,r-s} - \frac{\lambda}{2}\big(a_{r-1+s,r-1-s} + a_{r+1+s,r+1-s} - a_{r+s+1,r-s-1} - a_{r+s-1,r-s+1}\big), \tag{2.66}$$

which can be rewritten as

$$i\hbar \frac{da_{m,n}}{dt} = \hbar\omega n a_{m,n} - \frac{\lambda}{2}\big(a_{m-1,n-1} + a_{m+1,n+1} - a_{m+1,n-1} - a_{m-1,n+1}\big). \tag{2.67}$$

Notice that, if m and n have the same parity, then $m \pm 1$ and $n \pm 1$ also have the same parity.

For the QP model, the only change is that $r - s$ is transformed into $r^2 - s^2$ and, in terms of m and n, this is

$$r^2 - s^2 = (r+s)(r-s) = mn. \tag{2.68}$$

Therefore, the equation for the Fourier coefficients in the case of the QP reads

$$i\hbar \frac{da_{m,n}}{dt} = \frac{\hbar^2}{2I} mn a_{m,n} - \frac{\lambda}{2}(a_{m-1,n-1} + a_{m+1,n+1} - a_{m+1,n-1} - a_{m-1,n+1}). \tag{2.69}$$

The final evolution equations

To write the final equations for $w(\theta, m, t)$, we simply multiply both sides of (2.67) and (2.69) by $\frac{1}{2\pi} e^{in\theta}$ and sum the equations for n of the same parity as m. For the SHR, using (2.63), we get on the left-hand side of (2.67)

$$\frac{1}{2\pi} \sum_{\substack{n \text{ same} \\ \text{parity as } m}} i\hbar \frac{da_{m,n}}{dt} e^{in\theta} = i\hbar \frac{\partial w}{\partial t}(\theta, m, t). \tag{2.70}$$

Again using (2.63), the first term on the right-hand side of (2.67) becomes

$$\frac{1}{2\pi}\sum_{\substack{n \text{ same} \\ \text{parity as } m}} \hbar\omega n a_{m,n} e^{in\theta} = -i\hbar\omega\frac{\partial w}{\partial\theta}(\theta,m,t), \tag{2.71}$$

whilst the second term becomes

$$\begin{aligned}-\frac{\lambda}{4\pi}\sum_{\substack{n \text{ same} \\ \text{parity as } m}} a_{m-1,n-1}e^{in\theta} &= -\frac{\lambda}{4\pi}e^{i\theta}\sum_{\substack{n \text{ same} \\ \text{parity as } m}} a_{m-1,n-1}e^{i(n-1)\theta} = -\frac{\lambda}{4\pi}e^{i\theta}\sum_{\substack{n \text{ same} \\ \text{parity as } m-1}} a_{m-1,n}e^{in\theta} \\ &= -\frac{\lambda}{2}e^{i\theta}w(\theta,m-1,t),\end{aligned} \tag{2.72}$$

and similarly for the other terms

$$\begin{aligned}&-\frac{\lambda}{4\pi}\sum_{\substack{n \text{ same} \\ \text{parity as } m}} (a_{m+1,n+1} - a_{m+1,n-1} - a_{m-1,n+1})e^{in\theta} \\ &= -\frac{\lambda}{2}[e^{-i\theta}w(\theta,m+1,t) - e^{i\theta}w(\theta,m+1,t) - e^{-i\theta}w(\theta,m-1,t)].\end{aligned} \tag{2.73}$$

Putting (2.67) and (2.70)–(2.73) together, we get

$$\begin{aligned}i\hbar\frac{\partial w}{\partial t}(\theta,m,t) = &-i\hbar\omega\frac{\partial w}{\partial\theta}(\theta,m,t) - \frac{\lambda}{2}[e^{i\theta}w(\theta,m-1,t) + e^{-i\theta}w(\theta,m+1,t) - \\ &- e^{i\theta}w(\theta,m+1,t) - e^{-i\theta}w(\theta,m-1,t)],\end{aligned} \tag{2.74}$$

which is equivalent to

$$\boxed{\hbar\frac{\partial w}{\partial t}(\theta,m,t) = -\hbar\omega\frac{\partial w}{\partial\theta}(\theta,m,t) - \lambda\sin(\theta)[w(\theta,m-1,t) - w(\theta,m+1,t)].} \tag{2.75}$$

For the QP, the only change is in the first term on the right-hand side. From (2.69) the factor n in (2.71) becomes mn and

$$\frac{1}{2\pi}\sum_{\substack{n \text{ same} \\ \text{parity as } m}} mna_{m,n}e^{in\theta} = -im\frac{\partial w}{\partial\theta}(\theta,m,t), \tag{2.76}$$

so that the final equation for the QP is

$$\boxed{\hbar\frac{\partial w}{\partial t}(\theta,m,t) = -\frac{\hbar^2}{2I}m\frac{\partial w}{\partial\theta}(\theta,m,t) - \lambda\sin(\theta)[w(\theta,m-1,t) - w(\theta,m+1,t)].} \tag{2.77}$$

2.4.3 The Evolution equation from the Moyal bracket

In [2] Bizarro computed the evolution equation starting from the differential form of the Moyal bracket $[h,w]_\star$. In this section it will be seen that starting from the integral form (2.50) for the Moyal product the same result can be achieved in a much easier way.

We start with the Wigner transform of the Quantum Pendulum Hamiltonian (2.47). Given that the Moyal bracket is bilinear we can compute separately the contributions from the kinetic energy and the potential energy and then add them.

The Kinetic term

Starting with the kinetic energy and using (2.50) and (2.45) with $f(l) = l^2/2I$:

$$h_1 \bigstar w(\theta, m) = \frac{\hbar^2}{8\pi^2 I} \int_0^{2\pi} d\theta' \int_0^{2\pi} d\theta'' \sum_{\substack{m',m'':\\ m'+m''\text{ same}\\ \text{parity as } m \text{ and}\\ m+m' \text{ even}}} \left(\tfrac{m+m'}{2}\right)^2 w(\theta + \theta'', m + m'') e^{i(\theta' m'' - \theta'' m')}. \quad (2.78)$$

Notice that the conditions on m' and m'' imply that m' has the same parity as m and that m'' is even. Integrating in θ' only the term $m'' = 0$ survives

$$h_1 \bigstar w(\theta, m) = \frac{\hbar^2}{4\pi I} \int_0^{2\pi} d\theta'' \sum_{\substack{m' \text{ same}\\ \text{parity as } m}} \left(\tfrac{m+m'}{2}\right)^2 w(\theta + \theta'', m) e^{-i\theta'' m'}. \quad (2.79)$$

Defining a new variable $\bar{\theta} = \theta + \theta''$ we can write

$$h_1 \bigstar w(\theta, m) = \frac{\hbar^2}{4\pi I} \sum_{\substack{m' \text{ same}\\ \text{parity as } m}} e^{im'\theta} \int_0^{2\pi} d\bar{\theta} \left(\tfrac{m+m'}{2}\right)^2 w(\bar{\theta}, m) e^{-i\bar{\theta} m'}, \quad (2.80)$$

and similarly

$$w \bigstar h_1(\theta, m) = \frac{\hbar^2}{4\pi I} \sum_{\substack{m'' \text{ same}\\ \text{parity as } m}} e^{-im''\theta} \int_0^{2\pi} d\bar{\theta} \left(\tfrac{m+m''}{2}\right)^2 w(\bar{\theta}, m) e^{i\bar{\theta} m''}. \quad (2.81)$$

It is now time to expand the powers $(m + m')^2$ and $(m + m'')^2$. Doing so, it is immediate that the terms with m^2 in $h_1 \bigstar w$ and $w \bigstar h_1$ are identical if we identity the variables m' with $-m''$. This means that they cancel in $[h, w]_\bigstar$. For the terms with $2mm'$ and m'^2 we notice that

$$m' e^{-i\bar{\theta} m'} = i \frac{\partial}{\partial \bar{\theta}} e^{-i\bar{\theta} m'} \quad (2.82)$$

and so we can integrate by parts the terms with m' once and the terms with m'^2 twice. In the latter case we obtain

$$-\frac{\hbar^2}{16\pi I} \sum_{\substack{m' \text{ same}\\ \text{parity as } m}} e^{im'\theta} \int_0^{2\pi} d\bar{\theta} \frac{\partial^2 w}{\partial \bar{\theta}^2}(\bar{\theta}, m) e^{-i\bar{\theta} m'} \quad (2.83)$$

for $h_1 \bigstar w$ and the same term with $m'' = -m'$ in $w \bigstar h_1$. Again, this means that they cancel in $[h, w]_\bigstar$. The only terms that survive are the ones linear in m'

$$-i \frac{\hbar^2 m}{8\pi I} \sum_{\substack{m' \text{ same}\\ \text{parity as } m}} e^{im'\theta} \int_0^{2\pi} d\bar{\theta} \frac{\partial w}{\partial \bar{\theta}}(\bar{\theta}, m) e^{-i\bar{\theta} m'} = -i \frac{\hbar^2 m}{8\pi I} \int_0^{2\pi} d\bar{\theta} \frac{\partial w}{\partial \bar{\theta}}(\bar{\theta}, m) \left(\sum_{\substack{m' \text{ same}\\ \text{parity as } m}} e^{im'(\theta - \bar{\theta})} \right). \quad (2.84)$$

Inside the brackets we see from (2.1) that we have the expression for a combination of the periodic delta functions $\check{\delta}(\theta-\bar{\theta})$ and $\check{\delta}(\theta-\bar{\theta}+\pi)$. Therefore, we get

$$-i\frac{\hbar^2 m}{8I}\left(\frac{\partial w}{\partial\theta}(\theta,m)+(-1)^m\frac{\partial w}{\partial\theta}(\theta+\pi,m)\right) \tag{2.85}$$

in $h_1\bigstar w$ and an equal term with $+i$ in $w\bigstar h_1$. So,

$$[h_1,w]_\bigstar(\theta,m)=-2i\frac{\hbar^2 m}{8I}\left(\frac{\partial w}{\partial\theta}(\theta,m)+(-1)^m\frac{\partial w}{\partial\theta}(\theta+\pi,m)\right)=-i\frac{\hbar^2 m}{2I}\frac{\partial w}{\partial\theta}(\theta,m), \tag{2.86}$$

where in the last equality we have used the fact that $w(\theta+\pi,m)=(-1)^m w(\theta,m)$. The last expression coincides with the Kinetic term in (2.77) (remember that we cancelled the imaginary factor i there).

The Potential term

Starting with the Potential energy and using (2.50) and (2.46) we have:

$$h_2\bigstar w(\theta,m)=\frac{-\lambda}{(2\pi)^2}\int_0^{2\pi}d\theta'\int_0^{2\pi}d\theta''\sum_{\substack{m',m'':\\ m'+m''\text{ same}\\ \text{parity as } m \text{ and}\\ m+m'\text{ odd}}}\cos(\theta+\theta')w(\theta+\theta'',m+m'')e^{i(\theta'm''-\theta''m')}. \tag{2.87}$$

We observe that the conditions on m' and m'' imply that m' has the same parity as $m\pm 1$ and that m'' is odd. Also, we can split the cosine as a sum of two complex exponentials. The complex exponentials in θ' are then of the form $e^{i\theta'(m''\pm1)}$, and when we integrate in θ' only the terms with $m''=\pm1$ survive. The remaining terms have the form

$$\frac{-\lambda}{4\pi}e^{\pm i\theta}\int_0^{2\pi}d\theta''\sum_{\substack{m'\text{ same}\\ \text{parity as } m\mp1}}w(\theta+\theta'',m\mp1)e^{-i\theta''m'}. \tag{2.88}$$

We can again identify the sum in m' has a combination of periodic delta functions and get

$$\begin{aligned}[h_2,w]_\bigstar(\theta,m)=&\frac{-\lambda}{2}\left(e^{i\theta}w(\theta,m-1)+e^{-i\theta}w(\theta,m+1)-e^{i\theta}w(\theta,m+1)-e^{i\theta}w(\theta,m-1)\right)\\ =&-\lambda i\sin(\theta)(w(\theta,m-1)-w(\theta,m+1)),\end{aligned} \tag{2.89}$$

which coincides with the Potential term in (2.77) (again, remember that we cancelled the imaginary factor i there).

2.5 Stationary States, Observables and the Helmholtz equation

In this section several generalities about states in the Density Operator representation will be reviewed.

2.5.1 Stationary states and observables

In the Density Operator representation a *state* $\hat{\rho}$ is a positive operator (hermitian with non-negative eigenvalues) of trace 1. An *observable* is any hermitian operator $\hat{A}$. The evolution equations for a state and an observable are the same, modulo a minus sign. This means that the equation for a *stationary* state or observable is the same, namely $[\hat{H}, \hat{A}] = 0$. In this thesis several families of solutions for the stationarity equation of the SHR and QP models will be given, both in the Wigner representation, that is $[h, a]_\star = 0$, and in the Density Operator representation.

Stationary pure states

Pure states are those states $\hat{\rho}$ that are determined by a wave function $|\psi\rangle$, meaning that they have the form $\hat{\rho} = |\psi\rangle\langle\psi|$. *Stationary* pure states are those pure states that correspond to eigenstates of the Hamiltonian, namely, $\hat{\rho} = |E\rangle\langle E|$, with $\hat{H}|E\rangle = E|E\rangle$.

There are two other characterizations of pure states. Both have a non-linearity involved. The first is the famous $\hat{\rho}^2 = \hat{\rho}$. The second involves the matrix elements of the operator. The matrix elements of a pure state in any basis $(e_i)_{i\in I}$ have the product form

$$\langle e_i|\hat{\rho}|e_j\rangle = C_i C_j^* \tag{2.90}$$

for some sequence of complex numbers $(C_i)_{i\in I}$, which sequence then gives the expansion of the wave function $|\psi\rangle$ in the basis $(e_i)_{i\in I}$, that is,

$$|\psi\rangle = \sum_{i\in I} C_i e_i. \tag{2.91}$$

The natural basis to deal with rotational problems is the angular-momentum basis, in which pure states are those states $\hat{\rho}$ whose matrix elements can be factored as

$$\langle r|\hat{\rho}|s\rangle = C_r C_s^*, \tag{2.92}$$

the sequence $(C_r)_{r\in\mathbb{Z}}$ then giving us the Fourier expansion of the wave function:

$$\psi(\theta) = \frac{1}{\sqrt{2\pi}} \sum_{r=-\infty}^{\infty} C_r e^{ir\theta}. \tag{2.93}$$

The evolution equation for an observable $\hat{A}(t)$ in the Heisenberg picture is

$$-i\hbar \frac{d\hat{A}}{dt} = [\hat{H}, \hat{A}] \tag{2.94}$$

or, equivalently, in the Wigner picture

$$-i\hbar \frac{\partial a}{\partial t} = [h, a]_\star, \tag{2.95}$$

a stationary observable being one such that $\hat{A}(t) \equiv \hat{A}$, that is, $d\hat{A}/dt = 0$ or, equivalently, one such that $\hat{H}$ commutes with $\hat{A}$, so their Wigner transforms $h(\theta, m)$ and $a(\theta, m)$ commute with respect to the Moyal bracket. Comparing (2.56) and (2.62) with (2.94) and (2.95), we see that stationary density operators (representing stationary states) and stationary observables are determined by the same equations, so the latter include the former and constitute the general outcome of solving an equation of the type $[h, a]_\star = 0$, or $\partial a/\partial t = 0$ as per (2.95).

Preliminaries on integral operators

The observables of relevance to experiment are functions of x and p, or in our case θ and l. This means that in general they will be unbounded operators. This, in principle, is not the case of the stationary operators that will be presented in this thesis. Nevertheless, I think the reader will not find them without interest. To better understand the following a brief review of integral operators is in order.

An *integral operator* $\hat{A}$ acts on a function ψ by

$$(\hat{A}\psi)(\theta) = \int d\theta' K(\theta, \theta')\psi(\theta') \tag{2.96}$$

where $K(\theta, \theta')$ is the *integral kernel* of $\hat{A}$. The matrix elements of $\hat{A}$ in the angular basis are given by the values of K:

$$\langle\theta_1|\hat{A}|\theta_2\rangle = K(\theta_1, \theta_2) \tag{2.97}$$

and the matrix elements in the angular momentum basis are given by the Fourier coefficients of K:

$$\langle r|\hat{A}|s\rangle = \frac{1}{2\pi}\int d\theta_1 d\theta_2 K(\theta_1, \theta_2)e^{-ir\theta_1}e^{is\theta_2} \tag{2.98}$$

so that

$$K(\theta_1, \theta_2) = \frac{1}{2\pi}\sum_{r,s}\langle r|\hat{A}|s\rangle e^{ir\theta_1}e^{-is\theta_2}. \tag{2.99}$$

Notice that an integral operator $\hat{A}$ is hermitian only if $K(\theta_1, \theta_2) = K(\theta_2, \theta_1)^*$ and that a pure state $\hat{\rho} = |\psi\rangle\langle\psi|$ is a particular case of an integral operator with $K(\theta_1, \theta_2) = \psi(\theta_1)\psi(\theta_2)^*$.

Restricting the Wigner transform to integral operators one can thus regard the Wigner transform as a map between functions of two angular variables $K(\theta_1, \theta_2)$ and phase-space functions $A(\theta, m)$ or $a(\theta, m)$.

Making the left-hand sides of (2.60) and (2.61) equal to zero, while replacing $\hat{\rho}_{r,s}$ with $\langle r|\hat{A}|s\rangle$, the resulting expressions can also be seen as an equation involving the Fourier coefficients of the integral kernel $K(\theta_1, \theta_2)$. From this equation a differential equation for $K(\theta_1, \theta_2)$ can be found. This leads us to our next topic.

2.5.2 The Quantum Pendulum and the Helmholtz equation

Setting to zero the left-hand side of (2.61), multiplying by $e^{ir\theta_1}e^{-is\theta_2}$, and summing over r and s, in a manner similar to what has been done in Sec. 2.4.2, one gets

$$\frac{\partial^2 K}{\partial\theta_1^2} - \frac{\partial^2 K}{\partial\theta_2^2} + \frac{2\lambda I}{\hbar^2}[\cos(\theta_1) - \cos(\theta_2)]K = 0 \tag{2.100}$$

Comparing this eq. with Helmholtz' equation in modified elliptic coordinates (check Eq. (2) in § 10.11 of [16])

$$\frac{\partial^2 u}{\partial z_1^2} - \frac{\partial^2 u}{\partial z_2^2} - \frac{\Omega^2}{2}[\cos(2z_1) - \cos(2z_2)]u = 0 \qquad (2.101)$$

ones finds that they are equivalent if $z_1 = \theta_1/2$, $z_2 = \theta_2/2$, and $\Omega^2 = -16\lambda I/\hbar^2$.

This implies that to obtain integral kernels of stationary observables one can first look at solutions of the 2d Helmholtz equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \Omega^2 u = 0 \qquad (2.102)$$

and then substitute x by $\cos(\theta_1/2)\cos(\theta_2/2)$ and y by $i\sin(\theta_1/2)\sin(\theta_2/2)$. If the resulting function has period 2π in θ_1 and θ_2 then we have a solution of (2.100). Reciprocally, given a solution to equation (2.100) for the integral kernel of a stationary operator then, by inverting the coordinate transformation, one obtains a solution to the Helmholtz equation in cartesian coordinates.

The 2d Helmholtz equation is actually the context where Mathieu functions first appeared. This equation is separable in four different orthogonal coordinate systems [23]: cartesian (x, y), polar (r, θ), elliptic (ξ, η) and parabolic (u, v). Its solutions being, respectively: products of exponential functions, product of Bessel function times exponential function, product of modified Mathieu function times Mathieu function and product of parabolic cylinder functions. The real and imaginary parts of these solutions are independent solutions. In all these cases the separated solutions form a basis of the space of solutions.

As a byproduct of our analysis, in this thesis we wil be able to write the solutions of the Helmholtz eq. in cartesian and polar coodinates into elliptic coordinates as series of products of exponentals $e^{r\xi}e^{is\eta}$, with r and s integers, in a closed form. It is possible that this is a new result.

The solutions of the Helmholtz eq. we will be looking at are: the solutions in cartesian coordinates $K(\theta_1, \theta_2) = u(x, y) = e^{i\omega x}e^{i\sqrt{\Omega^2-\omega^2}y}$ of period 2π, that is, of the form $K(\theta_1, \theta_2) = u(x, y) = \cos(\omega x)\cos(\sqrt{\Omega^2 - \omega^2}y)$ and $K(\theta_1, \theta_2) = u(x, y) = \sin(\omega x)\sin(\sqrt{\Omega^2 - \omega^2}y)$, where ω is a continuous parameter; and the solutions in polar coordinates of even index $K(\theta_1, \theta_2) = u(r, \phi) = J_{2p}(\Omega r)e^{\pm i2p\phi}$, where p is a nonnegative integer. These solutions can be divided into solutions that are even or odd as functions of θ_1 and θ_2. In particular, $K(\theta_1, \theta_2) = u(r, \phi) = J_{2p}(\Omega r)\cos(2p\phi)$ and $K(\theta_1, \theta_2) = u(r, \phi) = J_{2p}(\Omega r)\sin(2p\phi)$ generate the same space of functions as the products of Mathieu functions of even order $ce_{2n}(\theta_1/2)ce_{2n}(\theta_2/2)$ and $se_{2n}(\theta_1/2)se_{2n}(\theta_2/2)$, respectively. That is, they generate the same space of functions as the products of eigenfunctions of the Quantum Pendulum and so they generate the space of solutions to eq. (2.100) for the integral kernel of stationary operators.

As discussed in section 2.2.1, the Mathieu functions of even order are eigenstates of the QP model, but no closed forms are known for them. It would be interesting if the Wigner transform shed some new light on this problem. In section 4.3.2 it will be seen that it seems this may indeed be the case. Also, surprisingly, it also seems that to write the Fourier coefficients of the solutions of the Helmholtz eq. in cartesian and polar coordinates into modified elliptic coordinates in a closed form it is best to first compute their Wigner transforms and then their Fourier coefficients. These then give us immediately the

Fourier coefficients of the Helmholtz solutions using (2.42) and (2.99).

Chapter 3

Solutions of the Stationarity Equations - Wigner function

In this chapter, several families of Wigner transforms of stationary observables are presented, both for the Simplified Hindered Rotator and the Quantum Pendulum. In the first section we give the simplest solutions. In both sections 3.1 and 3.2 we start from the right-hand sides of (2.75) and (2.77), replacing $w(\theta, m)$ with $a(\theta, m)$, whereas in section 3.3 we work directly with the Fourier expansions of the Wigner transforms and start from the right-hand sides of (2.67) and (2.69). In section 3.4, the results of the previous sections will be compared looking for common solutions. In the final section, the Wigner transforms of integral kernels that satisfy the Helmholtz equation will be computed and compared with the solutions previously obtained.

3.1 Simplest solutions

Making the right-hand side of (2.75) equal to 0, after replacing $w(\theta, m)$ with $a(\theta, m)$, we have

$$\frac{\partial a}{\partial \theta}(\theta, m) = -\frac{\lambda}{\hbar\omega}\sin(\theta)[a(\theta, m-1) - a(\theta, m+1)], \tag{3.1}$$

and so, defining as Bizarro in [2], $y = 2(\lambda/\hbar\omega)\cos(\theta)$ and $Z(y, m) = a(\theta, m)$, we get

$$2\frac{\partial Z}{\partial y}(y, m) = Z(y, m-1) - Z(y, m+1) \tag{3.2}$$

for the SHR. In the case of the QP, the right-hand side of (2.77) gives

$$m\frac{\partial a}{\partial \theta}(\theta, m) = -2\frac{\lambda I}{\hbar^2}\sin(\theta)[a(\theta, m-1) - a(\theta, m+1)], \tag{3.3}$$

whence, putting $y = -2(\lambda I/\hbar^2)\cos(\theta)$ and $Z(y, m) = a(\theta, m)$,

$$m\frac{\partial Z}{\partial y}(y, m) = Z(y, m+1) - Z(y, m-1). \tag{3.4}$$

3.1.1 Continuous families of solutions

If we make the simple hypothesis that $Z(y,m)$ is of the form

$$Z(y,m) = e^{y} f(m), \tag{3.5}$$

where $f(m)$ is some function to be determined, then, factoring out e^{y}, we obtain an equation for $f(m)$ only. For our purposes, we can add an extra parameter to the expression for $Z(y,m)$:

$$Z(y,m) = e^{\alpha y} f(m). \tag{3.6}$$

The equations for the SHR and QP models become respectively:

$$\alpha 2 f(m) = f(m-1) - f(m+1) \tag{3.7}$$

and

$$\alpha m f(m) = f(m+1) - f(m-1). \tag{3.8}$$

Simplified Hindered Rotator

In the first case we have a second order difference equation with constant coefficients. The way to solve it (see [24]) is to suppose $f(m) = z^{m}$ and solve $2\alpha z = 1 - z^{2}$. That is, we have two linearly independent solutions

$$Z(y,m) = e^{\alpha y}(-\alpha \pm \sqrt{\alpha^{2}+1})^{m}. \tag{3.9}$$

The corresponding family of Wigner functions is given by linear combinations of

$$a(\theta,m) = e^{2\alpha(\lambda/\hbar\omega)\cos(\theta)}(-\alpha \pm \sqrt{\alpha^{2}+1})^{m}. \tag{3.10}$$

Not all these solutions are Wigner transforms of operators. From the definition (2.42) it is seen that if m is even then $a(\theta,m)$ has only even Fourier coefficients and if m is odd then $a(\theta,m)$ has only odd coefficients. Only the linear combinations that satisfy this condition are allowed. Hence, the family of stationary Wigner functions for the Simplified Hindered Rotator is given by

$$a_{\alpha}(\theta,m) = e^{2\alpha(\lambda/\hbar\omega)\cos(\theta)}(-\alpha \pm \sqrt{\alpha^{2}+1})^{m} + e^{-2\alpha(\lambda/\hbar\omega)\cos(\theta)}(+\alpha \mp \sqrt{\alpha^{2}+1})^{m}. \tag{3.11}$$

Notice that if $\alpha = 0$ then $a(\theta,2m) = 2$ and $a(\theta,2m+1) = 0$. This the most trivial solution, it is the Wigner transform of the identity operator $\hat{I}$ times 4π. It satisfies the stationarity equation as it should, since the identity always commutes with the Hamiltonian.

Quantum Pendulum

Here we must solve a second order difference equation with variable coefficents. Since the coefficient is a linear function of m it is useful to use generating functions, because we will then obtain a first order differential equation. That is, we suppose there is a function $h(z)$ such that

$$h(z) = \sum_{m=-\infty}^{+\infty} f(m) z^m, \tag{3.12}$$

and solve

$$\alpha z^2 h'(z) = h(z) - z^2 h(z). \tag{3.13}$$

The general solution of which is

$$h(z) = De^{\frac{-1}{\alpha}\left(\frac{1}{z}+z\right)}. \tag{3.14}$$

To obtain $f(m)$ we expand $h(z)$ with $D = 1$,

$$\begin{aligned} h(z) =& e^{\frac{-1}{\alpha}z^{-1}} e^{\frac{-1}{\alpha}z} = \left(\sum_{n=0}^{\infty}\left(\frac{-1}{\alpha}\right)^n \frac{1}{n!}z^{-n}\right)\left(\sum_{k=0}^{\infty}\left(\frac{-1}{\alpha}\right)^k \frac{1}{k!}z^k\right) \\ =& \sum_{m=-\infty}^{\infty} z^m \sum_{n=0}^{\infty} \frac{1}{n!(n+m)!}\left(\frac{-1}{\alpha}\right)^{m+2n}. \end{aligned} \tag{3.15}$$

Noticing that the last sum is similar to the power series expression for Bessel functions (A.22) we arrive at

$$f(m) = i^m J_m\left(\frac{2i}{\alpha}\right), \tag{3.16}$$

and

$$Z(y,m) = e^{\alpha y} i^m J_m\left(\frac{2i}{\alpha}\right). \tag{3.17}$$

The family of stationary Wigner functions for the Quantum Pendulum is then given by

$$\boxed{a_\alpha(\theta,m) = e^{-2\alpha(\lambda I/\hbar^2)\cos(\theta)} i^m J_m\left(\frac{2i}{\alpha}\right) + e^{2\alpha(\lambda I/\hbar^2)\cos(\theta)} i^m J_m\left(\frac{2i}{-\alpha}\right).} \tag{3.18}$$

3.2 Two discrete variables

3.2.1 The Simplified Hindered Rotator

In solving (3.2), and despite the fact that Bizarro [2] already noticed that Bessel functions provide a solution for it, it will be instructive to rederive this result without prior knowledge of the properties of Bessel functions. We start by writing $Z(y,m)$ as a power series:

$$Z(y,m) = \sum_{j=-\infty}^{\infty} X(m,j) y^j \tag{3.19}$$

and, equating terms in (3.2), we get an equation for $X(m,j)$:

$$2(j+1)X(m,j+1) = X(m-1,j) - X(m+1,j). \tag{3.20}$$

Coming now to the main trick to solve this type of equation, which is separation of variables [24], we assume that

$$X(m,j) = f(j-m)g(j+m) \tag{3.21}$$

and get

$$2(j+1)f(j+1-m)g(j+1+m) = f(j-m+1)g(j+m-1) - f(j-m-1)g(j+m+1). \tag{3.22}$$

Subsequently defining $n = j-m$ and $k = j+m$, we have $j = (n+k)/2$ and $m = (k-n)/2$, whence

$$(n+k+2)f(n+1)g(k+1) = f(n+1)g(k-1) - f(n-1)g(k+1) \tag{3.23}$$

and, dividing throughout by $f(n+1)g(k+1)$ and rearranging,

$$n+1+\frac{f(n-1)}{f(n+1)} = -k-1+\frac{g(k-1)}{g(k+1)}. \tag{3.24}$$

For (3.24) to be verified, both its sides must equal some constant D so that, from $D = n+1+f(n-1)/f(n+1)$, we get

$$f(n+2) = \frac{-1}{(n+2)-D}f(n), \tag{3.25}$$

a solution reading

$$f(n) = \frac{(-1)^{\frac{n}{2}}}{(n-D)!!}, \tag{3.26}$$

with $n!! = n(n-2)(n-4)...$, implying

$$f(n) = \frac{(-1)^{\frac{n}{2}}}{2^{\frac{n}{2}-d}\left(\frac{n}{2}-d\right)!} \tag{3.27}$$

if, for the sake of simplifying (3.26), we suppose that both n and D are even (meaning that $D = 2d$); and $f(n) = 0$, if n is odd. Since 2^d is a constant multiplier, and because the equation (3.25) we are trying to solve is linear (hence true when we multiply a solution by a constant), we can disregard this constant to obtain

$$f(n) = \frac{(-1)^{\frac{n}{2}}}{2^{\frac{n}{2}}\left(\frac{n}{2}-d\right)!}. \tag{3.28}$$

Similarly, from the right-hand side of (3.24) being equal to the same constant D, we get

$$g(k+2) = \frac{1}{k+2+D}\,g(k), \tag{3.29}$$

and the same reasoning gives us

$$g(k) = \frac{1}{2^{\frac{k}{2}}\left(\frac{k}{2}+d\right)!}, \tag{3.30}$$

when k is even, and $g(k) = 0$, otherwise.

Putting (3.28) and (3.30) together, and recalling (3.21), we have

$$X(m,j) = \frac{(-1)^{\frac{j-m}{2}}}{2^{\frac{j-m}{2}}\left(\frac{j-m}{2}-d\right)!}\frac{1}{2^{\frac{j+m}{2}}\left(\frac{j+m}{2}+d\right)!} = \frac{(-1)^{\frac{j-m}{2}}}{2^{j}\left(\frac{j-m}{2}-d\right)!\left(\frac{j+m}{2}+d\right)!} \tag{3.31}$$

for j and m of the same parity, which, substituted in (3.19), yields

$$Z(y,m) = \sum_{\substack{j \text{ same} \\ \text{parity as } m}} \frac{(-1)^{\frac{j-m}{2}}}{2^{j}\left(\frac{j-m}{2}-d\right)!\left(\frac{j+m}{2}+d\right)!} y^{j}, \tag{3.32}$$

so that we are now close to the form of a Bessel function. Recalling the relation between factorials and Euler's gamma function to make the convention that $(-n)! = \Gamma(-n-1) = \infty$ for n a positive integer, then $1/(-n)! = 0$ and we see that the only nonvanishing terms in the series (3.32) are those with $j \pm (m+2d) \geq 0$, that is, $j = |m+2d| + 2k$ with k a nonnegative integer. Therefore, modulo a constant multiplier,

$$Z(y,m) = (-1)^{mH(-m-2d)}\left(\frac{y}{2}\right)^{|m+2d|}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!(k+|m+2d|)!}\left(\frac{y}{2}\right)^{2k}, \tag{3.33}$$

where $H(-m-2d)$ stands for the Heaviside unit step function, whence

$$Z(y,m) = J_{m+2d}(y) \tag{3.34}$$

is a solution to (3.2), something that is well known (A.24). Finally, we have the following family of solutions to the stationarity equation for the SHR model:

$$a_{2d}(\theta,m) = J_{m+2d}\left(\frac{2\lambda}{\hbar\omega}\cos(\theta)\right). \tag{3.35}$$

Notice that, modulo the 2π factor, we had already met these solutions in (2.49).

3.2.2 The Quantum Pendulum

Wanting to solve (3.4), we again write $Z(y,m)$ as the power series (3.19), only this time $X(m,j)$ must satisfy the equation

$$m(j+1)X(m,j+1) = X(m+1,j) - X(m-1,j). \tag{3.36}$$

The solution is again obtained by separation of variables, but we now suppose the form

$$X(m,j) = f(j-m)g(j+m)h(j) \tag{3.37}$$

and, by making two different hypothesis about $h(j)$, we arrive at two different families of solutions. Substituting, we obtain

$$\begin{aligned} m(j+1)f(j+1-m)g(j+1+m)h(j+1) =& f(j-m-1)g(j+m+1)h(j)- \\ &- f(j-m+1)g(j+m-1)h(j). \end{aligned} \tag{3.38}$$

First discrete family.

Making the hypothesis that $(j+1)h(j+1) = 2h(j)$, for instance, $h(j) = 2^j/j!$, we get, after factoring out $h(j)$,

$$2mf(j+1-m)g(j+1+m) = f(j-m-1)g(j+m+1) - f(j-m+1)g(j+m-1). \tag{3.39}$$

Changing variables as we did for the SHR model,

$$(k-n)f(n+1)g(k+1) = f(n-1)g(k+1) - f(n+1)g(k-1), \tag{3.40}$$

and, again dividing by $f(n+1)g(k+1)$, we arrive at

$$k + \frac{g(k-1)}{g(k+1)} = n + \frac{f(n-1)}{f(n+1)}. \tag{3.41}$$

Adding 1 to both sides of (3.41) we see, as we did earlier, that

$$f(n) = \frac{(-1)^{\frac{n}{2}}}{2^{\frac{n}{2}}\left(\frac{n}{2}-d\right)!} \tag{3.42}$$

is a solution for n even, and that a similar result ensues for $g(k)$ with k even.

Going back to (3.37),

$$\begin{aligned} X(m,j) &= \frac{(-1)^{\frac{j-m}{2}}}{2^{\frac{j-m}{2}}\left(\frac{j-m}{2}-d\right)!} \frac{(-1)^{\frac{j+m}{2}}}{2^{\frac{j+m}{2}}\left(\frac{j+m}{2}-d\right)!} \frac{2^j}{j!} \\ &= \frac{(-1)^j}{\left(\frac{j-m}{2}-d\right)!\left(\frac{j+m}{2}-d\right)!j!} \end{aligned} \tag{3.43}$$

comes as a solution with j of the same parity as m and, substituting in (3.19), we arrive at

$$Z(y,m) = \sum_{\substack{j \text{ same} \\ \text{parity as } m}} \frac{(-1)^j}{\left(\frac{j-m}{2}-d\right)!\left(\frac{j+m}{2}-d\right)!j!} y^j. \tag{3.44}$$

Making the same remarks as before, and supposing moreover that d is nonnegative, we obtain

$$Z(y,m) = (-1)^m y^{|m|+2d} \sum_{k=0}^{\infty} \frac{1}{k!(k+|m|)!(2k+|m|+2d)!} y^{2k}. \tag{3.45}$$

The family of stationary solutions to the evolution equation for the QP model is then:

$$\boxed{a_{2d}(\theta,m)=\left(\tfrac{2\lambda I}{\hbar^2}\cos(\theta)\right)^{|m|+2d}{}_0\Psi_2\left(\left(|m|+1,1\right),\left(|m|+2d+1,2\right)\Big|\left(\tfrac{2\lambda I}{\hbar^2}\cos(\theta)\right)^2\right).} \tag{3.46}$$

Second discrete family.

Here we make the hypothesis $h(j+1)=4h(j)$, for example, $h(j)=4^j$, so, factoring out $h(j)$ in (3.38), we get

$$4m(j+1)f(j+1-m)g(j+1+m)=f(j-m-1)g(j+m+1)-f(j-m+1)g(j+m-1). \tag{3.47}$$

It is useful to do a translation $j\to j-1$,

$$4mjf(j-m)g(j+m)=f(j-m-2)g(j+m)-f(j-m)g(j+m-2), \tag{3.48}$$

so that, once again changing variables as we did previously,

$$(k-n)(k+n)f(n)g(k)=f(n-2)g(k)-f(n)g(k-2), \tag{3.49}$$

or, after dividing by $f(n)g(k)$:

$$k^2+\frac{g(k-2)}{g(k)}=n^2+\frac{f(n-2)}{f(n)}. \tag{3.50}$$

Since we have n^2 and k^2, instead of n and k as in (3.24) and (3.41), $f(n)$ and $g(k)$ are now given by two factorials. Writing the separation constant D as $D=4d^2$, we have

$$f(n)=\frac{-1}{n^2-D}f(n-2)=\frac{-1}{(n-2d)(n+2d)}f(n-2) \tag{3.51}$$

and, similarly to what we had before,

$$f(n)=\frac{(-1)^{\frac{n}{2}}}{2^n\left(\frac{n}{2}-d\right)!\left(\frac{n}{2}+d\right)!} \tag{3.52}$$

for n even. The expression for $g(k)$ is the same, so we can write

$$\begin{aligned}X(m,j)&=\frac{(-1)^{\frac{j-m}{2}}}{2^{j-m}\left(\frac{j-m}{2}-d\right)!\left(\frac{j-m}{2}+d\right)!}\cdot\frac{(-1)^{\frac{j+m}{2}}}{2^{j+m}\left(\frac{j+m}{2}-d\right)!\left(\frac{j+m}{2}+d\right)!}4^j\\&=\frac{(-1)^j}{\left(\frac{j-m}{2}-d\right)!\left(\frac{j-m}{2}+d\right)!\left(\frac{j+m}{2}-d\right)!\left(\frac{j+m}{2}+d\right)!}\end{aligned} \tag{3.53}$$

as a solution with j of the same parity as m. Substituting in (3.19):

$$Z(y,m)=\sum_{\substack{j\text{ same}\\\text{parity as }m}}\frac{(-1)^j}{\left(\frac{j-m}{2}-d\right)!\left(\frac{j-m}{2}+d\right)!\left(\frac{j+m}{2}-d\right)!\left(\frac{j+m}{2}+d\right)!}y^j \tag{3.54}$$

and, making the same reasoning as before,

$$Z(y,m) = (-1)^m y^{|m|+|2d|} \sum_{k=0}^{\infty} \frac{1}{k!(k+|2d|)!(k+|m|)!(k+|m|+|2d|)!} y^{2k}. \tag{3.55}$$

This gives the family:

$$\boxed{a_{2d}(\theta,m) = \left(\tfrac{2\lambda I}{\hbar^2}\cos(\theta)\right)^{|m|+|2d|} {}_0\Psi_3\left((|m|+1,1),(|2d|+1,1),(|m|+|2d|+1,1)\middle|\left(\tfrac{2\lambda I}{\hbar^2}\cos(\theta)\right)^2\right)} \tag{3.56}$$

of stationary solutions.

3.3 Three discrete variables

Instead of trying to solve equations (3.1) and (3.3) as in section 3.2, we work here directly with the Fourier coefficients of the Wigner transforms and equate the right-hand sides of (2.67) and (2.69) to 0. More precisely, we try to solve

$$\hbar\omega n a_{m,n} = \frac{\lambda}{2}(a_{m-1,n-1} + a_{m+1,n+1} - a_{m+1,n-1} - a_{m-1,n+1}) \tag{3.57}$$

or, defining the adimensional constant $c = -\lambda/2\hbar\omega$,

$$n a_{m,n} = -c(a_{m-1,n-1} + a_{m+1,n+1} - a_{m+1,n-1} - a_{m-1,n+1}). \tag{3.58}$$

for the SHR, whereas for the QP we try to solve

$$\frac{\hbar^2}{2I} mn a_{m,n} = \frac{\lambda}{2}(a_{m-1,n-1} + a_{m+1,n+1} - a_{m+1,n-1} - a_{m-1,n+1}), \tag{3.59}$$

or

$$mn a_{m,n} = -c(a_{m-1,n-1} + a_{m+1,n+1} - a_{m+1,n-1} - a_{m-1,n+1}), \tag{3.60}$$

if we define $c = -\lambda I/\hbar^2$.

3.3.1 The Simplified Hindered Rotator

As in 3.2, we expand the Fourier coefficients in a power series, but use the constants c instead of y:

$$a_{m,n} = \sum_{j\in\mathbb{Z}} Y(m,n,j) c^j, \tag{3.61}$$

so that, from (3.58), the equation for $Y(m,n,j)$ becomes

$$
\begin{aligned}
nY(m,n,j) = &- Y(m-1,n-1,j-1) - Y(m+1,n+1,j-1) \\
&+ Y(m+1,n-1,j-1) + Y(m-1,n+1,j-1).
\end{aligned} \tag{3.62}
$$

An important observation about this equation for $Y(m,n,j)$ is that its coefficients do not explicitly depend on m and j, which implies that, given a solution $Y(m,n,j)$, we immediately get a family of solutions by simply translating the original solution, that is, $Y_{m_0,j_0}(m,n,j) = Y(m+m_0,n,j+j_0)$ is also a solution. This property regarding j corresponds to the fact that we can multiply the solutions $a_{m,n}$ of (3.58) by a constant multiplier c^{-j_0}. The indepence regarding m is specific to the SHR model and will not be true of the QP model. We will therefore only consider translations in j. Translations in m will be implicit in the solutions that will be found.

Again as in 3.2, we now attempt to do separation of variables and assume that

$$
Y(m,n,j) = h(j+m)r(j-m)s(j+n)t(j-n)u(j). \tag{3.63}
$$

We also define the variables $k = j+m$, $l = j-m$, $p = j+n$, and $q = j-n$, which can be inverted to give $j = (k+l)/2 = (p+q)/2$, $m = (k-l)/2$, and $n = (p-q)/2$ so we can now write (3.62) as

$$
\begin{aligned}
nh(k)r(l)s(p)t(q)u(j) = &- h(k-2)r(l)s(p-2)t(q)u(j-1) - h(k)r(l-2)s(p)t(q-2)u(j-1) \\
&+ h(k)r(l-2)s(p-2)t(q)u(j-1) + h(k-2)r(l)s(p)t(q-2)u(j-1).
\end{aligned} \tag{3.64}
$$

Dividing by $h(k)r(l)s(p)t(q)$, we have

$$
nu(j) = -\left[\frac{h(k-2)s(p-2)}{h(k)s(p)} + \frac{r(l-2)t(q-2)}{r(l)t(q)} - \frac{r(l-2)s(p-2)}{r(l)s(p)} - \frac{h(k-2)t(q-2)}{h(k)t(q)}\right]u(j-1) \tag{3.65}
$$

First discrete family

Here we suppose that $u(j) = 4u(j-1)$, say, $u(j) = 4^j$, factor it out and substitute n for $(p-q)/2$ in (3.65) to get

$$
2(p-q) = -\frac{h(k-2)s(p-2)}{h(k)s(p)} - \frac{r(l-2)t(q-2)}{r(l)t(q)} + \frac{r(l-2)s(p-2)}{r(l)s(p)} + \frac{h(k-2)t(q-2)}{h(k)t(q)}, \tag{3.66}
$$

which accepts as solution

$$
1 = -\frac{h(k-2)}{h(k)}, \quad 1 = \frac{r(l-2)}{r(l)}, \quad p = \frac{s(p-2)}{s(p)}, \quad \text{and} \quad q = \frac{t(q-2)}{t(q)}. \tag{3.67}
$$

Hence, following the same methodology that led us to (3.28), (3.30), (3.42), and (3.52),

$$
h(k) = (-1)^{\frac{k}{2}}, \quad r(l) \equiv 1, \quad s(p) = \frac{1}{2^{\frac{p}{2}}\left(\frac{p}{2}\right)!}, \quad \text{and} \quad t(q) = \frac{1}{2^{\frac{q}{2}}\left(\frac{q}{2}\right)!} \tag{3.68}
$$

for k, p and q even.

Putting it all together,

$$Y(m,n,j) = (-1)^{\frac{j+m}{2}} \frac{1}{2^{\frac{j+n}{2}} \left(\frac{j+n}{2}\right)!} \frac{1}{2^{\frac{j-n}{2}} \left(\frac{j-n}{2}\right)!} 4^j = \frac{(-1)^{\frac{j+m}{2}} 2^j}{\left(\frac{j+n}{2}\right)! \left(\frac{j-n}{2}\right)!} \tag{3.69}$$

for j with the same parity as m and n, (3.69) reading as the archetype for this family. To get its general form, we notice that $p-q = (p+d_2)-(q+d_2)$ in (3.66) for any integer d_2, so that the last two equalities in (3.68) become

$$s(p) = \frac{1}{2^{\frac{p}{2}} \left(\frac{p+d_2}{2}\right)!} \quad \text{and} \quad t(q) = \frac{1}{2^{\frac{q}{2}} \left(\frac{q+d_2}{2}\right)!}. \tag{3.70}$$

Remembering what we said following (3.62), we get the general form for this family:

$$Y_{j_0,d_2}(m,n,j) = \frac{(-1)^{\frac{j+j_0+m}{2}} 2^{j+j_0}}{\left(\frac{j+j_0+n+d_2}{2}\right)! \left(\frac{j+j_0-n+d_2}{2}\right)!} \tag{3.71}$$

for j of the same parity as j_0+n+d_2 (in practice, we just suppose j_0 and d_2 are even). This translates into the Fourier coefficients

$$a_{m,n} = (-1)^{\frac{|n|+m-d_2}{2}} 2^{j_0} (2c)^{|n|-j_0-d_2} \sum_{k=0}^{+\infty} \frac{(-1)^k (2c)^{2k}}{k! \big(k+|n|\big)!}. \tag{3.72}$$

If we ignore the constant multiplier $(-1)^{\frac{d_2}{2}} 2^{j_0} (2c)^{-j_0-d_2}$ we finally get

$$a^1_{m,n} = (-1)^{\frac{n+m}{2}} J_n \left(-\frac{2\lambda}{\hbar\omega} \right). \tag{3.73}$$

Note that this is not a true family of solutions, it is just one solution. We will nevertheless maintain the terminology since the corresponding solution for the QP model will be a true family and the following solutions to the SHR model will also be true families.

Second discrete family

We now assume that $u(j) = 8ju(j-1)$, for example, $u(j) = 8^j j!$, and do the substitutions $n = (p-q)/2$ and $j = (p+q)/2$ on the left-hand side of (3.65):

$$nu(j) = 8nju(j-1) = 2(p-q)(p+q)u(j-1) = 2(p^2-q^2)u(j-1). \tag{3.74}$$

Factoring out $u(j-1)$ in (3.65), we get the same right-hand side as in (3.66), while on the left-hand side we get $2(p^2-q^2)$ in place of $2(p-q)$, which leads to two factorials instead of just one, as in the second family of 3.2.2, and we find a solution with

$$1 = -\frac{h(k-2)}{h(k)}, \quad 1 = \frac{r(l-2)}{r(l)}, \quad p^2 = \frac{s(p-2)}{s(p)}, \quad \text{and} \quad q^2 = \frac{t(q-2)}{t(q)}. \tag{3.75}$$

In the general case, noticing that $2(p^2-q^2)=2[(p^2-d_2^2)-(q^2-d_2^2)]$ for any integer d_2,

$$p^2-d_2^2=(p+d_2)(p-d_2)=\frac{s(p-2)}{s(p)} \quad \text{and} \quad q^2-d_2^2=(q+d_2)(q-d_2)=\frac{t(q-2)}{t(q)} \tag{3.76}$$

will also give a solution. Again, as before,

$$h(k)=(-1)^{\frac{k}{2}}, \quad r(l)\equiv 1, \quad s(p)=\frac{1}{2^p\left(\frac{p+d_2}{2}\right)!\left(\frac{p-d_2}{2}\right)!}, \quad \text{and} \quad t(q)=\frac{1}{2^q\left(\frac{q+d_2}{2}\right)!\left(\frac{q-d_2}{2}\right)!} \tag{3.77}$$

The general form for this family is thus

$$Y_{j_0,d_2}(m,n,j)=\frac{(-1)^{\frac{j+j_0+m}{2}}2^{j+j_0}(j+j_0)!}{\left(\frac{j+j_0+n+d_2}{2}\right)!\left(\frac{j+j_0+n-d_2}{2}\right)!\left(\frac{j+j_0-n+d_2}{2}\right)!\left(\frac{j+j_0-n-d_2}{2}\right)!}, \tag{3.78}$$

with j of the same parity as j_0+n+d_2 (again, in practice, we suppose that j_0 and d_2 are even). We should also make the convention that $Y_{j_0,d_2}(m,n,j)=0$ when $j+j_0$ is negative which, thinking in terms of Euler's gamma function, is always the case if $j+j_0$ has the same parity as $n+d_2$. Once again ignoring the global c^{-j_0} factor, the Fourier coefficients are of the form

$$a^{2,d_2}_{m,n}=(-1)^{\frac{n+m+d_2}{2}}(2c)^{|n|+|d_2|}\sum_{k=0}^{+\infty}\frac{(-1)^k\big(2k+|n|+|d_2|\big)!(2c)^{2k}}{k!\big(k+|n|\big)!\big(k+|d_2|\big)!\big(k+|n|+|d_2|\big)!}, \tag{3.79}$$

or

$$a^{2,d_2}_{m,n}=(-1)^{\frac{n+m+d_2}{2}}\left(-\frac{\lambda}{\hbar\omega}\right)^{|n|+|d_2|}{}_1\Psi_3\left(\begin{matrix}(|n|+|d_2|+1,2) & - & - \\ (|n|+1,1) & (|d_2|+1,1) & (|n|+|d_2|+1,1)\end{matrix}\middle| -\left(\frac{\lambda}{\hbar\omega}\right)^2\right). \tag{3.80}$$

Third discrete family

Here the reasoning is entirely analogous to the one for the second family, the only changes being that, instead of substituting j with $(p+q)/2$, we substitute it with $(k+l)/2$ and we further suppose that $u(j)=4ju(j-1)$, so that on the left-hand side of (3.65) we get

$$nu(j)=(p-q)(k+l)u(j-1)=(pk+pl-qk-ql)u(j-1). \tag{3.81}$$

Looking at the right-hand side of (3.65), we see that we get a solution if

$$k=-\frac{h(k-2)}{h(k)}, \quad l=\frac{r(l-2)}{r(l)}, \quad p=\frac{s(p-2)}{s(p)}, \quad \text{and} \quad q=\frac{t(q-2)}{t(q)}. \tag{3.82}$$

The general case for this family is achieved by taking notice that

$$(p-q)(k+l)=[(p+d_2)-(q+d_2)][(k+d_1)+(l-d_1)], \tag{3.83}$$

implying that

$$h(k)=\frac{(-1)^{\frac{k}{2}}}{2^{\frac{k}{2}}\big(\frac{k+d_1}{2}\big)!},\quad r(l)=\frac{1}{2^{\frac{l}{2}}\big(\frac{l-d_1}{2}\big)!},\quad s(p)=\frac{1}{2^{\frac{p}{2}}\big(\frac{p+d_2}{2}\big)!},\quad \text{and}\quad t(q)=\frac{1}{2^{\frac{q}{2}}\big(\frac{q+d_2}{2}\big)!} \tag{3.84}$$

is a solution as well.

Finally, the general form for this family reads

$$Y_{j_0,d_1,d_2}(m,n,j)=\frac{(-1)^{\frac{j+j_0+m}{2}}(j+j_0)!}{\big(\frac{j+j_0+m+d_1}{2}\big)!\big(\frac{j+j_0-m-d_1}{2}\big)!\big(\frac{j+j_0+n+d_2}{2}\big)!\big(\frac{j+j_0-n+d_2}{2}\big)!}, \tag{3.85}$$

with j of the same parity as j_0+m+d_1 and j_0+n+d_2, so that it is necessary to assume that d_1 and d_2 have the same parity (in practice, both will be even). To write the Fourier coefficients we must divide into cases. The first is when $|m+d_1|\geq|n|-d_2$:

$$a^{3,d_1,d_2}_{m,n}=(-1)^{\frac{|m+d_1|+m}{2}}c^{|m+d_1|}\sum_{k=0}^{+\infty}\frac{(-1)^k\big(2k+|m+d_1|\big)!(2c)^{2k}}{k!\big(k+|m+d_1|\big)!\big(k+\frac{|m+d_1|+|n|+d_2}{2}\big)!\big(k+\frac{|m+d_1|-|n|+d_2}{2}\big)!}. \tag{3.86}$$

The second, when $|n|-d_2\geq|m+d_1|$:

$$a^{3,d_1,d_2}_{m,n}=(-1)^{\frac{|n|+m-d_2}{2}}c^{|n|-d_2}\sum_{k=0}^{+\infty}\frac{(-1)^k\big(2k+|n|-d_2\big)!(2c)^{2k}}{k!\big(k+|n|\big)!\big(k+\frac{|n|-d_2+|m+d_1|}{2}\big)!\big(k+\frac{|n|-d_2-|m+d_1|}{2}\big)!}. \tag{3.87}$$

Or

$$a^{3,d_1,d_2}_{m,n}=\left(\frac{\lambda}{2\hbar\omega}\right)^{|m+d_1|}\sum_{k=0}^{+\infty}\frac{\big(2k+|m+d_1|\big)!\left(-\big(\frac{\lambda}{\hbar\omega}\big)^2\right)^k}{k!\big(k+|m+d_1|\big)!\big(k+\frac{|m+d_1|+|n|+d_2}{2}\big)!\big(k+\frac{|m+d_1|-|n|+d_2}{2}\big)!}, \tag{3.88}$$

when $|m+d_1|\geq|n|-d_2$ and

$$a^{3,d_1,d_2}_{m,n}=(-1)^{\frac{3|n|+m+d_1-3d_2}{2}}\left(\frac{\lambda}{2\hbar\omega}\right)^{|n|-d_2}\sum_{k=0}^{+\infty}\frac{\big(2k+|n|-d_2\big)!\left(-\big(\frac{\lambda}{\hbar\omega}\big)^2\right)^k}{k!\big(k+|n|\big)!\big(k+\frac{|n|-d_2+|m+d_1|}{2}\big)!\big(k+\frac{|n|-d_2-|m+d_1|}{2}\big)!} \tag{3.89}$$

when $|n|-d_2\geq|m+d_1|$.

Fourth discrete family

We now combine the previous two families, put $u(j)=8j^2u(j-1)$, and substitute one j with $(k+l)/2$ and the other with $(p+q)/2$, so that on the left-hand side of (3.65) we have

$$nu(j)=(p-q)(k+l)(p+q)u(j-1)=(p^2-q^2)(k+l)u(j-1)=(p^2k+p^2l-q^2k-q^2l)u(j-1). \tag{3.90}$$

Looking again at the right-hand side of (3.65), we see that we have a solution provided that

$$k=-\frac{h(k-2)}{h(k)},\quad l=\frac{r(l-2)}{r(l)},\quad p^2=\frac{s(p-2)}{s(p)},\quad \text{and}\quad q^2=\frac{t(q-2)}{t(q)},\tag{3.91}$$

the general case for this family following from observing that

$$(p^2-q^2)(k+l)=[(p^2-d_2^2)-(q^2-d_2^2)][(k+d_1)+(l-d_1)],\tag{3.92}$$

so that we still get a solution if we set

$$k+d_1=-\frac{h(k-2)}{h(k)},\quad l-d_1=\frac{r(l-2)}{r(l)},\quad p^2-d_2^2=(p+d_2)(p-d_2)=\frac{s(p-2)}{s(p)},\quad \text{and}$$
$$q^2-d_2^2=(q+d_2)(q-d_2)=\frac{t(q-2)}{t(q)}.\tag{3.93}$$

The general, final form for this family becomes

$$Y_{j_0,d_1,d_2}(m,n,j)=\frac{(-1)^{\frac{j+j_0+m}{2}}(j+j_0)!(j+j_0)!}{\left(\frac{j+j_0+m+d_1}{2}\right)!\left(\frac{j+j_0-m-d_1}{2}\right)!\left(\frac{j+j_0+n+d_2}{2}\right)!\left(\frac{j+j_0+n-d_2}{2}\right)!\left(\frac{j+j_0-n+d_2}{2}\right)!\left(\frac{j+j_0-n-d_2}{2}\right)!},\tag{3.94}$$

with j of the same parity as j_0+m+d_1 and j_0+n+d_2. To write the Fourier coefficients the first case is $|m+d_1|\geq|n|+|d_2|$:

$$a^{4,d_1,d_2}_{m,n}=(-1)^{\frac{|m+d_1|+m}{2}}c^{|m+d_1|}\sum_{k=0}^{+\infty}\frac{(-1)^k\big(2k+|m+d_1|\big)!\big(2k+|m+d_1|\big)!}{k!\big(k+|m+d_1|\big)!\big(k+\frac{|m+d_1|+|n|+|d_2|}{2}\big)!\big(k+\frac{|m+d_1|+|n|-|d_2|}{2}\big)!}$$
$$\times\frac{(2c)^{2k}}{\big(k+\frac{|m+d_1|-|n|+|d_2|}{2}\big)!\big(k+\frac{|m+d_1|-|n|-|d_2|}{2}\big)!},\tag{3.95}$$

The second case is $|n|+|d_2|\geq|m+d_1|$:

$$a^{4,d_1,d_2}_{m,n}=(-1)^{\frac{|n|+m+|d_2|}{2}}c^{|n|+|d_2|}\sum_{k=0}^{+\infty}\frac{(-1)^k\big(2k+|n|+|d_2|\big)!\big(2k+|n|+|d_2|\big)!}{k!\big(k+|n|\big)\big(k+|d_2|\big)!\big(k+|n|+|d_2|\big)!}$$
$$\times\frac{(2c)^{2k}}{\big(k+\frac{|n|+|d_2|+|m+d_1|}{2}\big)!\big(k+\frac{|n|+|d_2|-|m+d_1|}{2}\big)!},\tag{3.96}$$

Or

$$a^{4,d_1,d_2}_{m,n}=\left(\frac{\lambda}{2\hbar\omega}\right)^{|m+d_1|}\sum_{k=0}^{+\infty}\frac{\big(2k+|m+d_1|\big)!\big(2k+|m+d_1|\big)!}{k!\big(k+|m+d_1|\big)!\big(k+\frac{|m+d_1|+|n|+|d_2|}{2}\big)!\big(k+\frac{|m+d_1|+|n|-|d_2|}{2}\big)!}$$
$$\times\frac{\Big(-\big(\frac{\lambda}{\hbar\omega}\big)^2\Big)^k}{\big(k+\frac{|m+d_1|-|n|+|d_2|}{2}\big)!\big(k+\frac{|m+d_1|-|n|-|d_2|}{2}\big)!},\tag{3.97}$$

when $|m+d_1| \geq |n|+|d_2|$ and

$$a^{4,d_1,d_2}_{m,n} = (-1)^{\frac{3|n|+m+d_1+3|d_2|}{2}} \left(\frac{\lambda}{2\hbar\omega}\right)^{|n|+|d_2|} \sum_{k=0}^{+\infty} \frac{\big(2k+|n|+|d_2|\big)!\big(2k+|n|+|d_2|\big)!}{k!\big(k+|n|\big)\big(k+|d_2|\big)!\big(k+|n|+|d_2|\big)!} \times \frac{\Big(-\big(\frac{\lambda}{\hbar\omega}\big)^2\Big)^k}{\big(k+\frac{|n|+|d_2|+|m+d_1|}{2}\big)!\big(k+\frac{|n|+|d_2|-|m+d_1|}{2}\big)!}, \tag{3.98}$$

when $|n|+|d_2| \geq |m+d_1|$.

3.3.2 The Quantum Pendulum

For the QP, expanding again the Fourier coefficients $a_{m,n}$ in a power series, and comparing (3.58) with (3.60), we see that the only difference from (3.62) will be that we now have mn on the left-hand side instead of n:

$$\begin{aligned} mnY(m,n,j) = &-Y(m-1,n-1,j-1) - Y(m+1,n+1,j-1) \\ &+ Y(m+1,n-1,j-1) + Y(m-1,n+1,j-1). \end{aligned} \tag{3.99}$$

The same separation of variables as in (3.63) gives the same expression as (3.65), except for mn replacing n on the left-hand side:

$$mnu(j) = -\left[\frac{h(k-2)s(p-2)}{h(k)s(p)} + \frac{r(l-2)t(q-2)}{r(l)t(q)} - \frac{r(l-2)s(p-2)}{r(l)s(p)} - \frac{h(k-2)t(q-2)}{h(k)t(q)}\right] u(j-1). \tag{3.100}$$

First discrete family

We set $m=(k-l)/2$ and $n=(p-q/)2$, suppose additionally that $u(j)=-4u(j-1)$, for instance, $u(j)=(-4)^j$, and obtain, after factoring out $u(j-1)$ in (3.100):

$$-(kp-kq-lp+lq) = -\frac{h(k-2)s(p-2)}{h(k)s(p)} - \frac{r(l-2)t(q-2)}{r(l)t(q)} + \frac{r(l-2)s(p-2)}{r(l)s(p)} + \frac{h(k-2)t(q-2)}{h(k)t(q)}, \tag{3.101}$$

so the solution

$$k = \frac{h(k-2)}{h(k)}, \quad l = \frac{r(l-2)}{r(l)}, \quad p = \frac{s(p-2)}{s(p)}, \quad \text{and} \quad q = \frac{t(q-2)}{t(q)} \tag{3.102}$$

follows. In the general case we remark that

$$mn = \frac{[(k+d_1)-(l+d_1)][(p+d_2)-(q+d_2))]}{4} \tag{3.103}$$

for any d_1 and d_2, which means that

$$h(k) = \frac{1}{2^{\frac{k}{2}}\left(\frac{k+d_1}{2}\right)!}, \quad r(l) = \frac{1}{2^{\frac{l}{2}}\left(\frac{l+d_1}{2}\right)!}, \quad s(p) = \frac{1}{2^{\frac{p}{2}}\left(\frac{p+d_2}{2}\right)!}, \quad \text{and} \quad t(q) = \frac{1}{2^{\frac{q}{2}}\left(\frac{q+d_2}{2}\right)!} \tag{3.104}$$

also do the job.

The general form for this family is then

$$Y_{j_0,d_1,d_2}(m,n,j) = \frac{(-1)^{j+j_0}}{\left(\frac{j+j_0+m+d_1}{2}\right)!\left(\frac{j+j_0-m+d_1}{2}\right)!\left(\frac{j+j_0+n+d_2}{2}\right)!\left(\frac{j+j_0-n+d_2}{2}\right)!}, \tag{3.105}$$

with j of the same parity as j_0+m+d_1 and j_0+n+d_2, as before. The Fourier coefficients when $|m|-d_1 \geq |n|-d_2$ are:

$$a^{1,d_1,d_2}_{m,n} = (-c)^{|m|-d_1} \sum_{k=0}^{+\infty} \frac{c^{2k}}{k!\left(k+|m|\right)!\left(k+\frac{|m|-d_1+|n|+d_2}{2}\right)!\left(k+\frac{|m|-d_1-|n|+d_2}{2}\right)!}, \tag{3.106}$$

and when $|n|-d_2 \geq |m|-d_1$:

$$a^{1,d_1,d_2}_{m,n} = (-c)^{|n|-d_2} \sum_{k=0}^{+\infty} \frac{c^{2k}}{k!\left(k+|n|\right)!\left(k+\frac{|n|-d_2+|m|+d_1}{2}\right)!\left(k+\frac{|n|-d_2-|m|+d_1}{2}\right)!}. \tag{3.107}$$

Or

$$\boxed{a^{1,d_1,d_2}_{m,n} = \left(\frac{\lambda I}{\hbar^2}\right)^{|m|-d_1} {}_0\Psi_3\left((|m|+1,1), \left(\tfrac{|m|-d_1+|n|+d_2+2}{2},1\right), \left(\tfrac{|m|-d_1-|n|+d_2+2}{2},1\right) \middle| \left(\frac{\lambda I}{\hbar^2}\right)^2\right),} \tag{3.108}$$

when $|m|-d_1 \geq |n|-d_2$ and

$$\boxed{a^{1,d_1,d_2}_{m,n} = \left(\frac{\lambda I}{\hbar^2}\right)^{|n|-d_2} {}_0\Psi_3\left((|n|+1,1), \left(\tfrac{|n|-d_2+|m|+d_1+2}{2},1\right), \left(\tfrac{|n|-d_2-|m|+d_1+2}{2},1\right) \middle| \left(\frac{\lambda I}{\hbar^2}\right)^2\right),} \tag{3.109}$$

when $|n|-d_2 \geq |m|-d_1$.

Second discrete family

Here we assume that $u(j) = -8ju(j-1)$ as in, for example, $u(j) = (-8)^j j!$, and replace j with $(k+l)/2$; then the left-hand side of (3.100) becomes

$$mnu(j) = -(k-l)(p-q)(k+l)u(j-1) = -(k^2-l^2)(p-q)u(j-1), \tag{3.110}$$

and we have a solution if

$$k^2 = \frac{h(k-2)}{h(k)}, \quad l^2 = \frac{r(l-2)}{r(l)}, \quad p = \frac{s(p-2)}{s(p)}, \quad \text{and} \quad q = \frac{t(q-2)}{t(q)}. \tag{3.111}$$

For the general case we write

$$(k^2-l^2)(p-q)=[(k^2-d_1^2)-(l^2-d_1^2)][(p+d_2)-(q+d_2)], \tag{3.112}$$

so that

$$k^2-d_1^2=(k+d_1)(k-d_1)=\frac{h(k-2)}{h(k)}, \quad l^2-d_1^2=(l+d_1)(l-d_1)=\frac{r(l-2)}{r(l)},$$
$$p+d_2=\frac{s(p-2)}{s(p)}, \quad \text{and} \quad q+d_2=\frac{t(q-2)}{t(q)} \tag{3.113}$$

also work, whence

$$h(k)=\frac{1}{2^k\left(\frac{k+d_1}{2}\right)!\left(\frac{k-d_1}{2}\right)!}, \quad r(l)=\frac{1}{2^l\left(\frac{l+d_1}{2}\right)!\left(\frac{l-d_1}{2}\right)!}, \quad s(p)=\frac{1}{2^{\frac{p}{2}}\left(\frac{p+d_2}{2}\right)!}, \quad \text{and} \quad t(q)=\frac{1}{2^{\frac{q}{2}}\left(\frac{q+d_2}{2}\right)!}. \tag{3.114}$$

Using the latter, we get the general form for this family

$$Y_{j_0,d_1,d_2}(m,n,j)=\frac{(-1)^{j+j_0}(j+j_0)!}{\left(\frac{j+j_0+m+d_1}{2}\right)!\left(\frac{j+j_0+m-d_1}{2}\right)!\left(\frac{j+j_0-m+d_1}{2}\right)!\left(\frac{j+j_0-m-d_1}{2}\right)!\left(\frac{j+j_0+n+d_2}{2}\right)!\left(\frac{j+j_0-n+d_2}{2}\right)!}, \tag{3.115}$$

with j of the same parity as j_0+m+d_1 and j_0+n+d_2.

The Fourier coefficients when $|m|+|d_1|\geq|n|-d_2$ are:

$$a_{m,n}^{2,d_1,d_2}=(-c)^{|m|+|d_1|}\sum_{k=0}^{+\infty}\frac{(2k+|m|+|d_1|)!}{k!(k+|m|)!(k+|d_1|)!(k+|m|+|d_1|)!\left(k+\frac{|m|+|d_1|+|n|+d_2}{2}\right)!} \times\frac{c^{2k}}{\left(k+\frac{|m|+|d_1|-|n|+d_2}{2}\right)!}, \tag{3.116}$$

and when $|n|-d_2\geq|m|+|d_1|$:

$$a_{m,n}^{2,d_1,d_2}=(-c)^{|n|-d_2}\sum_{k=0}^{+\infty}\frac{(2k+|n|-d_2)!}{k!(k+|n|)!\left(k+\frac{|n|-d_2+|m|+|d_1|}{2}\right)!\left(k+\frac{|n|-d_2+|m|-|d_1|}{2}\right)!} \times\frac{c^{2k}}{\left(k+\frac{|n|-d_2-|m|+|d_2|}{2}\right)!\left(k+\frac{|n|-d_2-|m|-|d_2|}{2}\right)!}. \tag{3.117}$$

Or

$$\boxed{a_{m,n}^{2,d_1,d_2}=\left(\frac{\lambda I}{\hbar^2}\right)^{|m|+|d_1|}\sum_{k=0}^{+\infty}\frac{(2k+|m|+|d_1|)!}{k!(k+|m|)!(k+|d_1|)!(k+|m|+|d_1|)!\left(k+\frac{|m|+|d_1|+|n|+d_2}{2}\right)!} \times\frac{\left(\frac{\lambda I}{\hbar^2}\right)^{2k}}{\left(k+\frac{|m|+|d_1|-|n|+d_2}{2}\right)!},} \tag{3.118}$$

when $|m| + |d_1| \geq |n| - d_2$ and

$$\boxed{\begin{aligned} a^{2,d_1,d_2}_{m,n} = \left(\frac{\lambda I}{\hbar^2}\right)^{|n|-d_2} \sum_{k=0}^{+\infty} & \frac{(2k+|n|-d_2)!}{k!(k+|n|)!\big(k+\frac{|n|-d_2+|m|+|d_1|}{2}\big)!\big(k+\frac{|n|-d_2+|m|-|d_1|}{2}\big)!} \\ & \times \frac{\big(\frac{\lambda I}{\hbar^2}\big)^{2k}}{\big(k+\frac{|n|-d_2-|m|+|d_2|}{2}\big)!\big(k+\frac{|n|-d_2-|m|-|d_2|}{2}\big)!}, \end{aligned}} \tag{3.119}$$

when $|n| - d_2 \geq |m| + |d_1|$.

Third discrete family

This is as the previous family but for the substitution of j with $(p+q)/2$ instead of $(k+l)/2$, so the left-hand side of (3.100) becomes

$$mnu(j) = -(k-l)(p-q)(p+q)u(j-1) = -(k-l)(p^2-q^2)u(j-1), \tag{3.120}$$

which admits a solution when

$$k = \frac{h(k-2)}{h(k)}, \quad l = \frac{r(l-2)}{r(l)}, \quad p^2 = \frac{s(p-2)}{s(p)}, \quad \text{and} \quad q^2 = \frac{t(q-2)}{t(q)}. \tag{3.121}$$

We notice that

$$(k-l)(p^2-q^2) = [(k+d_1)-(l+d_1)][(p^2-d_2^2)-(q^2-d_2^2)], \tag{3.122}$$

implying that

$$\begin{aligned} & k+d_1 = \frac{h(k-2)}{h(k)}, \quad l+d_1 = \frac{r(l-2)}{r(l)}, \quad p^2-d_2^2 = (p+d_2)(p-d_2) = \frac{s(p-2)}{s(p)}, \quad \text{and} \\ & q^2-d_2^2 = (q+d_2)(q-d_2) = \frac{t(q-2)}{t(q)} \end{aligned} \tag{3.123}$$

again also work, and thus we get

$$h(k) = \frac{1}{2^{\frac{k}{2}}\big(\frac{k+d_1}{2}\big)!}, \quad r(l) = \frac{1}{2^{\frac{l}{2}}\big(\frac{l+d_1}{2}\big)!}, \quad s(p) = \frac{1}{2^p\big(\frac{p+d_2}{2}\big)!\big(\frac{p-d_2}{2}\big)!}, \quad \text{and} \quad t(q) = \frac{1}{2^q\big(\frac{q+d_2}{2}\big)!\big(\frac{q-d_2}{2}\big)!}. \tag{3.124}$$

This leads us to the general form for this family, which reads

$$Y_{j_0,d_1,d_2}(m,n,j) = \frac{(-1)^{j+j_0}(j+j_0)!}{\big(\frac{j+j_0+m+d_1}{2}\big)!\big(\frac{j+j_0-m+d_1}{2}\big)!\big(\frac{j+j_0+n+d_2}{2}\big)!\big(\frac{j+j_0+n-d_2}{2}\big)!\big(\frac{j+j_0-n+d_2}{2}\big)!\big(\frac{j+j_0-n-d_2}{2}\big)!}, \tag{3.125}$$

if j is of the same parity as j_0+m+d_1 and j_0+n+d_2.

The Fourier coefficients when $|m|-d_1 \geq |n|+|d_2|$ are:

$$a_{m,n}^{3,d_1,d_2} = (-c)^{|m|-d_1} \sum_{k=0}^{+\infty} \frac{(2k+|m|-d_1)!}{k!(k+|m|)!\big(k+\frac{|m|-d_1+|n|+|d_2|}{2}\big)!\big(k+\frac{|m|-d_1+|n|-|d_2|}{2}\big)!} \times \frac{c^{2k}}{\big(k+\frac{|m|-d_1-|n|+|d_2|}{2}\big)!\big(k+\frac{|m|-d_1-|n|-|d_2|}{2}\big)!}, \tag{3.126}$$

and when $|n|+|d_2| \geq |m|-d_1$:

$$a_{m,n}^{3,d_1,d_2} = (-c)^{|n|+|d_2|} \sum_{k=0}^{+\infty} \frac{(2k+|n|+|d_2|)!}{k!(k+|n|)!(k+|d_2|)!(k+|n|+|d_2|)!\big(k+\frac{|n|+|d_2|+|m|+d_1}{2}\big)!} \times \frac{c^{2k}}{\big(k+\frac{|n|-d_2-|m|+d_1}{2}\big)!}. \tag{3.127}$$

Or

$$\boxed{a_{m,n}^{3,d_1,d_2} = \left(\frac{\lambda I}{\hbar^2}\right)^{|m|-d_1} \sum_{k=0}^{+\infty} \frac{(2k+|m|-d_1)!}{k!(k+|m|)!\big(k+\frac{|m|-d_1+|n|+|d_2|}{2}\big)!\big(k+\frac{|m|-d_1+|n|-|d_2|}{2}\big)!} \times \frac{\big(\frac{\lambda I}{\hbar^2}\big)^{2k}}{\big(k+\frac{|m|-d_1-|n|+|d_2|}{2}\big)!\big(k+\frac{|m|-d_1-|n|-|d_2|}{2}\big)!},} \tag{3.128}$$

when $|m|-d_1 \geq |n|+|d_2|$ and

$$\boxed{a_{m,n}^{3,d_1,d_2} = \left(\frac{\lambda I}{\hbar^2}\right)^{|n|+|d_2|} \sum_{k=0}^{+\infty} \frac{(2k+|n|+|d_2|)!}{k!(k+|n|)!(k+|d_2|)!(k+|n|+|d_2|)!\big(k+\frac{|n|+|d_2|+|m|+d_1}{2}\big)!} \times \frac{\big(\frac{\lambda I}{\hbar^2}\big)^{2k}}{\big(k+\frac{|n|-d_2-|m|+d_1}{2}\big)!},} \tag{3.129}$$

when $|n|+|d_2| \geq |m|-d_1$.

Fourth discrete family

We now assume that $u(j) = -16j^2u(j-1)$, as with $u(j) = (-16)^j j!j!$, and the left-hand side of (3.100) becomes

$$mnu(j) = -(k-l)(p-q)(k+l)(p+q)u(j-1) = -(k^2-l^2)(p^2-q^2)u(j-1), \tag{3.130}$$

so we can set as solution

$$k^2 = \frac{h(k-2)}{h(k)}, \quad l^2 = \frac{r(l-2)}{r(l)}, \quad p^2 = \frac{s(p-2)}{s(p)}, \quad \text{and} \quad q^2 = \frac{t(q-2)}{t(q)}. \tag{3.131}$$

Moving to the general case, we remark that

$$(k^2-l^2)(p^2-q^2) = [(k^2-d_1^2)-(l^2-d_1^2)][(p-d_2^2)-(q^2-d_2^2)], \tag{3.132}$$

so

$$k^2 - d_1^2 = (k+d_1)(k-d_1) = \frac{h(k-2)}{h(k)}, \quad l^2 - d_1^2 = (l+d_1)(l-d_1) = \frac{r(l-2)}{r(l)},$$
$$p^2 - d_2^2 = (p+d_2)(p-d_2) = \frac{s(p-2)}{s(p)}, \quad \text{and} \quad q^2 - d_2^2 = (q+d_2)(q-d_2) = \frac{t(q-2)}{t(q)}, \tag{3.133}$$

which leads us to get

$$h(k) = \frac{1}{2^k\left(\frac{k+d_1}{2}\right)!\left(\frac{k-d_1}{2}\right)!}, \quad r(l) = \frac{1}{2^l\left(\frac{l+d_1}{2}\right)!\left(\frac{l-d_1}{2}\right)!},$$
$$s(p) = \frac{1}{2^p\left(\frac{p+d_2}{2}\right)!\left(\frac{p-d_2}{2}\right)!}, \quad \text{and} \quad t(q) = \frac{1}{2^q\left(\frac{q+d_2}{2}\right)!\left(\frac{q-d_2}{2}\right)!}. \tag{3.134}$$

Assembling all this in (3.63), we arrive at the fourth family of solutions for the Fourier coefficients of stationary observables within the QP model:

$$\begin{aligned} Y_{j_0,d_1,d_2}(m,n,j) =& \frac{(-1)^{j+j_0}(j+j_0)!(j+j_0)!}{\left(\frac{j+j_0+m+d_1}{2}\right)!\left(\frac{j+j_0+m-d_1}{2}\right)!\left(\frac{j+j_0-m+d_1}{2}\right)!\left(\frac{j+j_0-m-d_1}{2}\right)!} \\ &\times \frac{1}{\left(\frac{j+j_0+n+d_2}{2}\right)!\left(\frac{j+j_0+n-d_2}{2}\right)!\left(\frac{j+j_0-n+d_2}{2}\right)!\left(\frac{j+j_0-n-d_2}{2}\right)!}, \end{aligned} \tag{3.135}$$

with j of the same parity as $j_0 + m + d_1$ and $j_0 + n + d_2$.

The Fourier coefficients when $|m| + |d_1| \geq |n| + |d_2|$ are:

$$\begin{aligned} a^{4,d_1,d_2}_{m,n} = (-c)^{|m|-d_1} \sum_{k=0}^{+\infty} & \frac{(2k+|m|+|d_1|)!(2k+|m|+|d_1|)!}{k!(k+|m|)!(k+|d_1|)!(k+|m|+|d_1|)!\left(k+\frac{|m|+|d_1|+|n|+|d_2|}{2}\right)!} \\ &\times \frac{c^{2k}}{\left(k+\frac{|m|+|d_1|+|n|-|d_2|}{2}\right)!\left(k+\frac{|m|+|d_1|-|n|+|d_2|}{2}\right)!\left(k+\frac{|m|+|d_1|-|n|-|d_2|}{2}\right)!}, \end{aligned} \tag{3.136}$$

and when $|n| + |d_2| \geq |m| + |d_1|$:

$$\begin{aligned} a^{4,d_1,d_2}_{m,n} = (-c)^{|n|+|d_2|} \sum_{k=0}^{+\infty} & \frac{(2k+|n|+|d_2|)!(2k+|n|+|d_2|)!}{k!(k+|n|)!(k+|d_2|)!(k+|n|+|d_2|)!\left(k+\frac{|n|+|d_2|+|m|+|d_1|}{2}\right)!} \\ &\times \frac{c^{2k}}{\left(k+\frac{|n|+|d_2|+|m|-|d_1|}{2}\right)!\left(k+\frac{|n|+|d_2|-|m|+|d_1|}{2}\right)!\left(k+\frac{|n|-d_2-|m|-|d_1|}{2}\right)!}. \end{aligned} \tag{3.137}$$

Or

$$\boxed{\begin{aligned} a^{4,d_1,d_2}_{m,n} = \left(\frac{\lambda I}{\hbar^2}\right)^{|m|-d_1} \sum_{k=0}^{+\infty} & \frac{(2k+|m|+|d_1|)!(2k+|m|+|d_1|)!}{k!(k+|m|)!(k+|d_1|)!(k+|m|+|d_1|)!\left(k+\frac{|m|+|d_1|+|n|+|d_2|}{2}\right)!} \\ &\times \frac{\left(\frac{\lambda I}{\hbar^2}\right)^{2k}}{\left(k+\frac{|m|+|d_1|+|n|-|d_2|}{2}\right)!\left(k+\frac{|m|+|d_1|-|n|+|d_2|}{2}\right)!\left(k+\frac{|m|+|d_1|-|n|-|d_2|}{2}\right)!}, \end{aligned}} \tag{3.138}$$

when $|m| + |d_1| \geq |n| + |d_2|$ and

$$\boxed{\begin{aligned} a^{4,d_1,d_2}_{m,n} = \left(\frac{\lambda I}{\hbar^2}\right)^{|n|+|d_2|} \sum_{k=0}^{+\infty} & \frac{(2k+|n|+|d_2|)!(2k+|n|+|d_2|)!}{k!(k+|n|)!(k+|d_2|)!(k+|n|+|d_2|)!\big(k+\frac{|n|+|d_2|+|m|+|d_1|}{2}\big)!} \\ & \times \frac{\left(\frac{\lambda I}{\hbar^2}\right)^{2k}}{\big(k+\frac{|n|+|d_2|+|m|-|d_1|}{2}\big)!\big(k+\frac{|n|+|d_2|-|m|+|d_1|}{2}\big)!\big(k+\frac{|n|-d_2-|m|-|d_1|}{2}\big)!}, \end{aligned}} \tag{3.139}$$

when $|n| + |d_2| \geq |m| + |d_1|$.

3.4 Comparisons between approaches

The continuous families of solutions of section 3.1 are not comparable to the discrete families of solutions in sections 3.2 and 3.3, except for special values of the parameter α. Consider, for example, the continuous family of section 3.1.1. If in (3.11) we set $\alpha = -i$, then taking into consideration the formula for the generating function of Bessel functions (A.26), one sees that the Fourier coefficients $a_{m,n}$ of this solution have the form $2i^{m+n}J_n(4c)$ for m and n of the same parity. This is the solution (3.73) in the first discrete family of solutions of the SHR.

To compare the solutions obtained via the two approaches detailed in sections 3.2 and 3.3, we only have to calculate their Fourier coefficients and subsequently write them as power series in the parameters $c = -\lambda/2\hbar\omega$, for the SHR model, or $c = -\lambda I/\hbar^2$, for the QP model. Recalling that we have set, in section 3.2, $a(\theta, m) = Z[-4c\cos(\theta), m]$ for the SHR and $a(\theta, m) = Z[2c\cos(\theta), m]$ for the QP, $a(\theta, m)$ is a periodic function in θ (for fixed m), and we now ascertain which are its Fourier coefficients. To do this, we need to first calculate the contributions of each power of $2\cos(\theta)$, which gives:

$$[2\cos(\theta)]^n = \left(e^{i\theta} + e^{-i\theta}\right)^n = \sum_{l=0}^{n} \binom{n}{l} e^{i(n-2l)\theta}. \tag{3.140}$$

3.4.1 The Simplified Hindered Rotator

We have, from the Bessel series expansion (3.33),

$$a(\theta, m) = Z[-4c\cos(\theta), m] = \sum_{j=0}^{\infty} \frac{(-1)^j}{j!(j+m+2d)!}[-2c\cos(\theta)]^{2j+m+2d} \tag{3.141}$$

for the solution found in section 3.2.1 or, making use of (3.140),

$$a(\theta, m) = \sum_{j=0}^{\infty} \frac{(-1)^j}{j!(j+m+2d)!}(-c)^{2j+m+2d} \sum_{l=0}^{2j+m+2d} \binom{2j+m+2d}{l} e^{i(2j+m+2d-2l)\theta}. \tag{3.142}$$

It is worth noticing that the generic $n = 2j+m+2d-2l$ in the exponential factor $e^{in\theta}$ appearing in (3.142) has the same parity as m, in accordance with the general expression (2.42) for $a(\theta, m)$ (with the dummy variable m' replaced with n). We can check as well that $e^{in\theta}$ and $e^{-in\theta}$ have the same coefficients and that these are real, which is also expected given that the classical-like function $a(\theta, m)$ associated with the self-adjoint quantum operator $\hat{A}$ must be real, as follows from (2.42). Lastly, we observe from (3.140) and (3.141) that c and $\cos(\theta)$ appear always with the same power and that the lowest power of $\cos(\theta)$ contributing to some $e^{in\theta}$ has exponent $|n|$, so $e^{in\theta}$ in (3.142) collects contributions of powers of c with exponents $2j+m+2d \geq |n|$. Now, making $n = 2j+m+2d-2l$, then $l = j+(m+2d-n)/2$ and the binomial coefficient becomes

$$\binom{2j+m+2d}{l} = \frac{(2j+m+2d)!}{l!(2j+m+2d-l)!} = \frac{\big(2j+m+2d\big)!}{\big(j+\frac{m+2d-n}{2}\big)!\big(j+\frac{m+2d+n}{2}\big)!}, \tag{3.143}$$

thus we have for the coefficient $a_{m,n}$ of the term in $e^{in\theta}$, with n of the same parity as m:

$$\frac{1}{2\pi}a_{m,n} = \sum_{j=0}^{\infty} \frac{(-1)^j(2j+m+2d)!}{j!(j+m+2d)!\big(j+\frac{m+2d-n}{2}\big)!\big(j+\frac{m+2d+n}{2}\big)!}(-c)^{2j+m+2d}. \tag{3.144}$$

As a result, setting $i = 2j+m+2d$ and thence $j = (i-m-2d)/2$:

$$\begin{aligned}\frac{1}{2\pi}a_{m,n} &= \sum_{\substack{i \text{ same} \\ \text{parity as } m}} \frac{(-1)^{\frac{i-m-2d}{2}}i!}{\big(\frac{i-m-2d}{2}\big)!\big(\frac{i+m+2d}{2}\big)!\big(\frac{i-n}{2}\big)!\big(\frac{i+n}{2}\big)!}(-c)^i \\ &= (-1)^d \sum_{\substack{i \text{ same} \\ \text{parity as } m}} \frac{(-1)^{\frac{i+m}{2}}i!}{\big(\frac{i-m-2d}{2}\big)!\big(\frac{i+m+2d}{2}\big)!\big(\frac{i-n}{2}\big)!\big(\frac{i+n}{2}\big)!}c^i,\end{aligned} \tag{3.145}$$

where we used the fact that i and m have the same parity to write $(-1)^i = (-1)^m$. Comparing this with the expressions already obtained for the different families of solutions, we see that it is a special case of the third family in section 3.3.1, defined via (3.85), with $j_0 = d_2 = 0$ and $d_1 = 2d$, and modulo a constant multiplier $(-1)^d 2\pi$.

3.4.2 The Quantum Pendulum

First discrete family

Putting together (3.45) and (3.140), the first family of solutions obtained in section 3.2.2 takes the form

$$\begin{aligned}a(\theta,m) &= Z[2c\cos(\theta), m] = \\ &= (-1)^m \sum_{j=0}^{\infty} \frac{1}{j!(j+|m|)!(2j+|m|+2d)!}c^{2j+|m|+2d} \sum_{l=0}^{2j+|m|+2d} \binom{2j+|m|+2d}{l} e^{i(2j+|m|+2d-2l)\theta},\end{aligned} \tag{3.146}$$

and, with $n = |m| + 2d + 2j - 2l$, the corresponding Fourier coefficient $a_{m,n}$ turns out to be:

$$\begin{aligned}\frac{1}{2\pi}a_{m,n} &= (-1)^m \sum_{j=0}^{\infty} \frac{1}{j!(j+|m|)!(2j+|m|+2d)!} \binom{2j+|m|+2d}{j+\frac{|m|+2d-n}{2}} c^{2j+|m|+2d} \\ &= (-1)^m \sum_{j=0}^{\infty} \frac{1}{j!(j+|m|)!\big(j+\frac{|m|+2d-n}{2}\big)!\big(j+\frac{|m|+2d+n}{2}\big)!} c^{2j+|m|+2d}, \end{aligned} \tag{3.147}$$

with n and m of the same parity.

If we now set $i = 2j + |m| + 2d$, we end up with

$$\frac{1}{2\pi}a_{m,n} = \sum_{\substack{i \text{ same} \\ \text{parity as } m}} \frac{(-1)^i}{\big(\frac{i-|m|-2d}{2}\big)!\big(\frac{i+|m|-2d}{2}\big)!\big(\frac{i-n}{2}\big)!\big(\frac{i+n}{2}\big)!} c^i, \tag{3.148}$$

where once more we used the fact that i and m are of the same parity, this being a solution that coincides, modulo the 2π factor, with the first family in section 3.3.2 when $j_0 = d_2 = 0$ and $d_1 = -2d$, as follows from comparison with (3.105).

Second discrete family

For the second family of solutions in section 3.2.2 we have, from (3.55) and (3.140):

$$\begin{aligned} a(\theta, m) =& (-1)^m \sum_{j=0}^{\infty} \frac{1}{j!(j+|2d|)!(j+|m|)!(j+|m|+|2d|)!} c^{2j+|m|+|2d|} \\ & \times \sum_{l=0}^{2j+|m|+|2d|} \binom{2j+|m|+|2d|}{l} e^{i(2j+|m|+|2d|-2l)\theta} \end{aligned} \tag{3.149}$$

With $n = 2j + |m| + |2d| - 2l$, then $l = j + (|m| + |2d| - n)/2$ and the binomial coefficient reads

$$\binom{2j+|m|+|2d|}{l} = \frac{(2j+|m|+|2d|)!}{l!(2j+|m|+|2d|-l)!} = \frac{(2j+|m|+|2d|)!}{\big(j+\frac{|m|+|2d|-n}{2}\big)!\big(j+\frac{|m|+|2d|+n}{2}\big)!}, \tag{3.150}$$

so that the Fourier coefficient $a_{m,n}$ for the generic term in $e^{in\theta}$, and for n of the same parity as m, is

$$\frac{a_{m,n}}{2\pi} = (-1)^m \sum_{j=0}^{\infty} \frac{(2j+|m|+|2d|)!}{j!(j+|2d|)!(j+|m|)!(j+|m|+|2d|)!\big(j+\frac{|m|+|2d|-n}{2}\big)!\big(j+\frac{|m|+|2d|+n}{2}\big)!} c^{2j+|m|+|2d|}. \tag{3.151}$$

Putting $i = 2j + |m| + |2d|$, so that $j = (i - |m| - |2d|)/2$, we finally get:

$$\frac{1}{2\pi}a_{m,n} = (-1)^m \sum_{\substack{i \text{ same} \\ \text{parity as } m}} \frac{i!}{\big(\frac{i-|m|-|2d|}{2}\big)!\big(\frac{i-|m|+|2d|}{2}\big)!\big(\frac{i+|m|-|2d|}{2}\big)!\big(\frac{i+|m|+|2d|}{2}\big)!\big(\frac{i-n}{2}\big)!\big(\frac{i+n}{2}\big)!} c^i, \tag{3.152}$$

or, noticing the expression above is symmetric in $|m|$ and $-|m|$,

$$\frac{1}{2\pi}a_{m,n} = (-1)^m \sum_{\substack{i \text{ same} \\ \text{parity as } m}} \frac{i!}{\left(\frac{i-m-|2d|}{2}\right)!\left(\frac{i-m+|2d|}{2}\right)!\left(\frac{i+m-|2d|}{2}\right)!\left(\frac{i+m+|2d|}{2}\right)!\left(\frac{i-n}{2}\right)!\left(\frac{i+n}{2}\right)!}c^i. \tag{3.153}$$

Going through the expressions given in section 3.3.2, we conclude that this corresponds to the particular case of the second family of solutions, as given by (3.115), for which $j_0 = d_2 = 0$ and $d_1 = 2d$.

3.5 Wigner transforms of Helmholtz solutions

Here the Wigner transforms of the integral kernels of stationary operators mentioned in section 2.5.2 are computed.

3.5.1 Family of cartesian solutions

Starting with the simplest solution in cartesian coordinates we make $K(\theta_1, \theta_2) = u(x, y) = \cos(\Omega x)$ and use $x = \cos(\theta_1/2)\cos(\theta_2/2)$, (2.43) and (2.97) to get

$$a(\theta, m) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta' e^{-im\theta'} K(\theta+\theta', \theta-\theta') \tag{3.154}$$

$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta' e^{-im\theta'} \cos\left(\Omega \cos\left(\tfrac{\theta+\theta'}{2}\right)\cos\left(\tfrac{\theta-\theta'}{2}\right)\right) \tag{3.155}$$

$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta' e^{-im\theta'} \cos\left(\tfrac{\Omega}{2}\left(\cos(\theta)+\cos(\theta')\right)\right) \tag{3.156}$$

Writing the outermost cosine in terms of complex exponentials, and recalling the form of the generating function for Bessel functions (A.26)

$$e^{i\beta\sin(\varphi)} = \sum_n J_n(\beta)e^{in\varphi}, \tag{3.157}$$

one gets

$$a(\theta, m) = \frac{1}{2}\left[i^m J_m\left(\frac{\Omega}{2}\right)e^{i\frac{\Omega}{2}\cos(\theta)} + i^m J_m\left(-\frac{\Omega}{2}\right)e^{-i\frac{\Omega}{2}\cos(\theta)}\right]. \tag{3.158}$$

Recalling that $\Omega^2 = -16\lambda I/\hbar^2$ we recognize in the expression inside square brackets the solution (3.18) of section 3.1.1 with $\alpha = i4/\Omega$.

In the general cases $K(\theta_1, \theta_2) = u(x, y) = \cos(\omega x)\cos(\sqrt{\Omega^2-\omega^2}y)$ and $K(\theta_1, \theta_2) = u(x, y) = \sin(\omega x)\sin(\sqrt{\Omega^2-\omega^2}y)$ we use additionally $y = i\sin(\theta_1/2)\sin(\theta_2/2)$ and get that the only difference from the previous case is that when we write the outermost cosines and sines in terms of complex exponentials and compute the Wigner transforms we get terms of the form

$$e^{i(\pm\omega\pm i\sqrt{\omega^2-\omega^2})\cos(\theta)}\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta' e^{-im\theta'} e^{i(\pm\omega\pm i\sqrt{\omega^2-\omega^2})\cos(\theta')}. \tag{3.159}$$

This means that the Wigner transforms are a linear combination of the two solutions in (3.18) with

$\alpha = 4(\pm\sqrt{\Omega^2 - \omega^2} + i\omega)/\Omega^2$.

3.5.2 Family of polar solutions

Here we study the Wigner transforms of the real and imaginary parts of $K(\theta_1, \theta_2) = u(r, \phi) = J_{2p}(\Omega r)e^{\pm i2p\phi}$. Beginning with the simplest case $p = 0$ and using (B.15), formula (3.154) becomes in this case

$$a(\theta, m) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta' e^{-im\theta'} J_0[\Omega\sqrt{\cos(\theta)\cos(\theta')}], \tag{3.160}$$

which, taking into consideration the power series form for the Bessel function (A.22), yields

$$a(\theta, m) = \sum_{k=0}^{\infty} \frac{(-\frac{\Omega^2}{4})^k \cos^k(\theta)}{k!k!} \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta' e^{-im\theta'} \cos^k(\theta') \tag{3.161}$$

or, taking into account (3.140)

$$a(\theta, m) = \sum_{\substack{k \text{ same} \\ \text{parity as } m}} \frac{(-\frac{\Omega^2}{4})^k \cos^k(\theta)}{2^k k!k!} \binom{k}{\frac{k-m}{2}} = \sum_{\substack{k \text{ same} \\ \text{parity as } m}} \frac{(-\frac{\Omega^2}{8})^k \cos^k(\theta)}{k!(\frac{k-m}{2})!(\frac{k+m}{2})!}. \tag{3.162}$$

Observing that $\Omega^2 = -16\lambda I/\hbar^2$ and that y in section 3.2.2 is defined by $y = -2(\lambda I/\hbar^2)\cos(\theta)$ we recognize in (3.162) the particular case with $d = 0$ of the first discrete family of solutions (3.44). Whence

$$a(\theta, m) = \left(-\frac{\Omega^2}{8}\cos(\theta)\right)^{|m|} \sum_{k=0}^{\infty} \frac{(-\frac{\Omega^2}{8})^{2k} \cos^{2k}(\theta)}{k!(k+|m|)!(2k+|m|)!}. \tag{3.163}$$

Moving on to the general case $p \geq 0$, with $K(\theta_1, \theta_2) = u(r, \phi) = J_{2p}(\Omega r)\cos(2p\phi)$, using (B.17) we have

$$a(\theta, m) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta' e^{-im\theta'} \frac{1}{2} J_{2p}[\Omega\sqrt{\cos(\theta)\cos(\theta')}] \left[\frac{\cos^p(\theta)}{\cos^p(\theta')} + \frac{\cos^p(\theta')}{\cos^p(\theta)}\right], \tag{3.164}$$

whence

$$a(\theta, m) = \frac{2^{4p-1}}{\Omega^{2p}} \sum_{\substack{k \text{ same} \\ \text{parity as } m}} \frac{(-\frac{\Omega^2}{8})^{k+2p} \cos^{k+2p}(\theta)}{(k+2p)!(\frac{k-m}{2})!(\frac{k+m}{2})!} + \frac{\Omega^{2p}}{2^{4p+1}} \sum_{\substack{k \text{ same} \\ \text{parity as } m}} \frac{(-\frac{\Omega^2}{8})^k \cos^k(\theta)}{k!(\frac{k-m}{2}+p)!(\frac{k+m}{2}+p)!}. \tag{3.165}$$

Comparing with the solutions of the first discrete family in section 3.2.2 we immediately see that the second series corresponds to (3.44) with $d = -p$. For the first series, making the translation $k \mapsto k + |m|$ we get (3.45) with $d = p$. So this Wigner transform is a linear combination of known solutions.

For $K(\theta_1, \theta_2) = u(r, \phi) = J_{2p}(\Omega r)\sin(2p\phi)$, using (B.19) we have

$$a(\theta, m) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta' e^{-im\theta'} \frac{i}{2} J_{2p}[\Omega\sqrt{\cos(\theta)\cos(\theta')}] \left[\frac{\cos^p(\theta')}{\cos^p(\theta)} - \frac{\cos^p(\theta)}{\cos^p(\theta')}\right], \tag{3.166}$$

which is the same as (3.164) except for the minus sign and the factor i. So, once again, we have a linear combination of known solutions, the first term is associated with the solution with $d = -p$ of the first discrete family in section 3.2.2 and the second term with the solution with $d = p$. Notice also that if we look at solutions of the Helmholtz solutions with complex exponentials $e^{i2\pi p\phi}$ and $e^{-i2\pi p\phi}$ then they are associated with Wigner stationarity solutions with $d = p$ and $d = -p$, respectively.

As a corollary to the above results we have that the first discrete family of section 3.2.2 is already a basis for the space of solutions of the stationarity equation, since the corresponding solutions of the 2d Helmholtz equation form a basis of the space generated by products of Mathieu functions of even order. That is, they form a basis of the space of functions $a(\theta, m)$ that commute with the Wigner transform of the Hamiltonian of the Quantum Pendulum (i.e., $[h, a]_\star = 0$).

Chapter 4

Solutions of the Stationarity Equations - Density Operator

In this chapter, several families of stationary observables are presented, both for the Simplified Hindered Rotator and the Quantum Pendulum, and their connections to stationary pure states are discussed. In the first section we give the matrix elements of stationary observables in the angular momentum basis. In the second section we study their relationship to solutions of the Helmholtz equation in elliptic coordinates. In the last section we discuss possible approaches to obtain closed forms for stationary pure states and hence to Mathieu functions.

4.1 Matrix elements of stationary observables

Making use of the notation $G(r,s,j)$ for the power-series coefficients of the matrix elements $\langle r|\hat{A}|s\rangle$, that is,

$$\langle r|\hat{A}|s\rangle = \sum_{j=-\infty}^{\infty} G(r,s,j)c^j, \tag{4.1}$$

and of equations (2.60) and (2.61) for the evolution of the density operator (with their left-hand sides set to zero), we obtain the following stationarity equations for $G(r,s,j)$:

$$(r-s)G(r,s,j) = -G(r-1,s,j-1) - G(r+1,s,j-1) + G(r,s+1,j-1) + G(r,s-1,j-1). \tag{4.2}$$

and

$$(r^2-s^2)G(r,s,j) = -G(r-1,s,j-1) - G(r+1,s,j-1) + G(r,s+1,j-1) + G(r,s-1,j-1), \tag{4.3}$$

pertaining, respectively, to the SHR and QP models.

One could try to solve the above equations by the procedure of section 3.3, by using separation of variables as in (3.63) and changing variables according to $m = r+s$ and $n = r-s$. The computations are exactly the same, and we will refrain from repeating them. In what follows only the relation $G(r,s,j) = Y(r+s, r-s, j)$ will be used, so we only present the final results. The main point here is that separation of variable turns out to be easier when working with the Wigner transform.

The reader should keep in mind what we said in section 2.5.1, that these matrix elements also correspond to the Fourier coefficients of their integral kernels $K(\theta_1, \theta_2)$, and this will be used in section 4.2.

4.1.1 The Simplified Hindered Rotator

From the above and (3.71), (3.78), (3.85), and (3.94), the four families of 3.3.1 give:

$$G^1_{j_0,d_2}(r,s,j) = \frac{(-1)^{\frac{j+j_0+r+s}{2}} 2^{j+j_0}}{\left(\frac{j+j_0+r-s+d_2}{2}\right)!\left(\frac{j+j_0-r+s+d_2}{2}\right)!}, \tag{4.4}$$

$$G^2_{j_0,d_2}(r,s,j) = \frac{(-1)^{\frac{j+j_0+r+s}{2}} 2^{j+j_0}(j+j_0)!}{\left(\frac{j+j_0+r-s+d_2}{2}\right)!\left(\frac{j+j_0+r-s-d_2}{2}\right)!\left(\frac{j+j_0-r+s+d_2}{2}\right)!\left(\frac{j+j_0-r+s-d_2}{2}\right)!}, \tag{4.5}$$

$$G^3_{j_0,d_1,d_2}(r,s,j) = \frac{(-1)^{\frac{j+j_0+r+s}{2}} (j+j_0)!}{\left(\frac{j+j_0+r+s+d_1}{2}\right)!\left(\frac{j+j_0-r-s-d_1}{2}\right)!\left(\frac{j+j_0+r-s+d_2}{2}\right)!\left(\frac{j+j_0-r+s+d_2}{2}\right)!}, \tag{4.6}$$

and

$$\begin{aligned} G^4_{j_0,d_1,d_2}(r,s,j) =& \frac{(-1)^{\frac{j+j_0+r+s}{2}} (j+j_0)!(j+j_0)!}{\left(\frac{j+j_0+r+s+d_1}{2}\right)!\left(\frac{j+j_0-r-s-d_1}{2}\right)!\left(\frac{j+j_0+r-s+d_2}{2}\right)!\left(\frac{j+j_0+r-s-d_2}{2}\right)!} \\ &\times \frac{1}{\left(\frac{j+j_0-r+s+d_2}{2}\right)!\left(\frac{j+j_0-r+s-d_2}{2}\right)!}, \end{aligned} \tag{4.7}$$

where j is of the same parity as $j_0+r+s+d_1$ and $G^i_{j_0,d_1,d_2}(r,s,j) = 0$, otherwise. Moreover, d_1 and d_2 are of the same parity in (4.6) and (4.7). Remembering the fact that $c = -\lambda/2\hbar\omega$ and recalling that the translations $j \mapsto j + j_0$ correspond to multiplying a solution by a global constant c^{-j_0} we can neglect the dependence in j_0 and write the matrix elements of the corresponding operators as

$$\langle r|\hat{A}^1_{d_2}|s\rangle = \sum_{\substack{j \text{ same} \\ \text{parity as} \\ r+s+d_2}} \frac{(-1)^{\frac{j+r+s}{2}}}{\left(\frac{j+r-s+d_2}{2}\right)!\left(\frac{j-r+s+d_2}{2}\right)!} \left(-\frac{\lambda}{\hbar\omega}\right)^j, \tag{4.8}$$

$$\langle r|\hat{A}^2_{d_2}|s\rangle = \sum_{\substack{j \text{ same} \\ \text{parity as} \\ r+s+d_2}} \frac{(-1)^{\frac{j+r+s}{2}} j!}{\left(\frac{j+r-s+d_2}{2}\right)!\left(\frac{j+r-s-d_2}{2}\right)!\left(\frac{j-r+s+d_2}{2}\right)!\left(\frac{j-r+s-d_2}{2}\right)!} \left(-\frac{\lambda}{\hbar\omega}\right)^j, \tag{4.9}$$

$$\langle r|\hat{A}^3_{d_1,d_2}|s\rangle = \sum_{\substack{j \text{ same} \\ \text{parity as} \\ r+s+d_1}} \frac{(-1)^{\frac{j+r+s}{2}} j!}{\left(\frac{j+r+s+d_1}{2}\right)!\left(\frac{j-r-s-d_1}{2}\right)!\left(\frac{j+r-s+d_2}{2}\right)!\left(\frac{j-r+s+d_2}{2}\right)!} \left(-\frac{\lambda}{2\hbar\omega}\right)^j, \tag{4.10}$$

and

$$\langle r|\hat{A}^4_{d_1,d_2}|s\rangle = \sum_{\substack{j \text{ same} \\ \text{parity as} \\ r+s+d_1}} \frac{(-1)^{\frac{j+r+s}{2}} j!j!}{\left(\frac{j+r+s+d_1}{2}\right)!\left(\frac{j-r-s-d_1}{2}\right)!\left(\frac{j+r-s+d_2}{2}\right)!\left(\frac{j+r-s-d_2}{2}\right)!\left(\frac{j-r+s+d_2}{2}\right)!\left(\frac{j-r+s-d_2}{2}\right)!} \left(-\frac{\lambda}{2\hbar\omega}\right)^j, \tag{4.11}$$

where d_1 and d_2 are of the same parity in (4.10) and (4.11). One should keep in mind that these are matrix elements of general stationary observables and not necessarily density matrices, they are not normalized, but, most importantly, they are probably not even positive operators.

4.1.2 The Quantum Pendulum

Similarly, from (3.105), (3.115), (3.125), and (3.135), we have for the four families of 3.3.2:

$$G^1_{j_0,d_1,d_2}(r,s,j) = \frac{(-1)^{j+j_0}}{\left(\frac{j+j_0+r+s+d_1}{2}\right)!\left(\frac{j+j_0-r-s+d_1}{2}\right)!\left(\frac{j+j_0+r-s+d_2}{2}\right)!\left(\frac{j+j_0-r+s+d_2}{2}\right)!}, \tag{4.12}$$

$$\begin{aligned} G^2_{j_0,d_1,d_2}(r,s,j) =& \frac{(-1)^{j+j_0}(j+j_0)!}{\left(\frac{j+j_0+r+s+d_1}{2}\right)!\left(\frac{j+j_0+r+s-d_1}{2}\right)!\left(\frac{j+j_0-r-s+d_1}{2}\right)!\left(\frac{j+j_0-r-s-d_1}{2}\right)!} \\ &\times \frac{1}{\left(\frac{j+j_0+r-s+d_2}{2}\right)!\left(\frac{j+j_0-r+s+d_2}{2}\right)!}, \end{aligned} \tag{4.13}$$

$$\begin{aligned} G^3_{j_0,d_1,d_2}(r,s,j) =& \frac{(-1)^{j+j_0}(j+j_0)!}{\left(\frac{j+j_0+r+s+d_1}{2}\right)!\left(\frac{j+j_0-r-s+d_1}{2}\right)!\left(\frac{j+j_0+r-s+d_2}{2}\right)!\left(\frac{j+j_0+r-s-d_2}{2}\right)!} \\ &\times \frac{1}{\left(\frac{j+j_0-r+s+d_2}{2}\right)!\left(\frac{j+j_0-r+s-d_2}{2}\right)!}, \end{aligned} \tag{4.14}$$

and

$$\begin{aligned} G^4_{j_0,d_1,d_2}(r,s,j) =& \frac{(-1)^{j+j_0}(j+j_0)!(j+j_0)!}{\left(\frac{j+j_0+r+s+d_1}{2}\right)!\left(\frac{j+j_0+r+s-d_1}{2}\right)!\left(\frac{j+j_0-r-s+d_1}{2}\right)!\left(\frac{j+j_0-r-s-d_1}{2}\right)!} \\ &\times \frac{1}{\left(\frac{j+j_0+r-s+d_2}{2}\right)!\left(\frac{j+j_0+r-s-d_2}{2}\right)!\left(\frac{j+j_0-r+s+d_2}{2}\right)!\left(\frac{j+j_0-r+s-d_2}{2}\right)!}, \end{aligned} \tag{4.15}$$

where j has the same parity as $j_0+r+s+d_1$ and $G^i_{j_0,d_1,d_2}(r,s,j) = 0$, otherwise. Moreover, d_1 and d_2 are of the same parity in (4.14) and (4.15). Recalling that $c = -\lambda I/\hbar^2$ and making the same observation as above about the j_0 parameter we can write the matrix elements of the corresponding operators as

$$\boxed{\langle r|\hat{A}^1_{d_1,d_2}|s\rangle = \sum_{\substack{j \text{ same} \\ \text{parity as} \\ r+s+d_1}} \frac{1}{\left(\frac{j+r+s+d_1}{2}\right)!\left(\frac{j-r-s+d_1}{2}\right)!\left(\frac{j+r-s+d_2}{2}\right)!\left(\frac{j-r+s+d_2}{2}\right)!}\left(\frac{\lambda I}{\hbar^2}\right)^j,} \tag{4.16}$$

$$\boxed{\langle r|\hat{A}^2_{d_1,d_2}|s\rangle = \sum_{\substack{j \text{ same} \\ \text{parity as} \\ r+s+d_1}} \frac{j!}{\left(\frac{j+r+s+d_1}{2}\right)!\left(\frac{j+r+s-d_1}{2}\right)!\left(\frac{j-r-s+d_1}{2}\right)!\left(\frac{j-r-s-d_1}{2}\right)!\left(\frac{j+r-s+d_2}{2}\right)!\left(\frac{j-r+s+d_2}{2}\right)!}\left(\frac{\lambda I}{\hbar^2}\right)^j,} \tag{4.17}$$

$$\boxed{\langle r|\hat{A}^3_{d_1,d_2}|s\rangle = \sum_{\substack{j \text{ same} \\ \text{parity as} \\ r+s+d_1}} \frac{j!}{\left(\frac{j+r+s+d_1}{2}\right)!\left(\frac{j-r-s+d_1}{2}\right)!\left(\frac{j+r-s+d_2}{2}\right)!\left(\frac{j+r-s-d_2}{2}\right)!\left(\frac{j-r+s+d_2}{2}\right)!\left(\frac{j-r+s-d_2}{2}\right)!}\left(\frac{\lambda I}{\hbar^2}\right)^j,} \tag{4.18}$$

and

$$\boxed{\begin{aligned}\langle r|\hat{A}^4_{d_1,d_2}|s\rangle = \sum_{\substack{j \text{ same} \\ \text{parity as} \\ r+s+d_1}} & \frac{j!j!}{\left(\frac{j+r+s+d_1}{2}\right)!\left(\frac{j+r+s-d_1}{2}\right)!\left(\frac{j-r-s+d_1}{2}\right)!\left(\frac{j-r-s-d_1}{2}\right)!\left(\frac{j+r-s+d_2}{2}\right)!\left(\frac{j+r-s-d_2}{2}\right)!} \\ & \times \frac{1}{\left(\frac{j-r+s+d_2}{2}\right)!\left(\frac{j-r+s-d_2}{2}\right)!}\left(\frac{\lambda I}{\hbar^2}\right)^j,\end{aligned}} \tag{4.19}$$

where d_1 and d_2 always of the same parity in (4.16)–(4.19).

4.1.3 Mellin Transform method

There is a method of solving the stationarity equations for the Density Operator and the Wigner function that includes the power series method, but that is more general: the Mellin transform method, reviewed in Appendix A.1. Defining a new function by considering the dependence of the matrix elements on the coupling constant c and doing a Mellin transform on the variable c

$$\tilde{B}(r,s;z) = \text{MT}[\langle r|\hat{A}|s\rangle(c);z] \tag{4.20}$$

and using property (A.18) that transforms a multiplication by c into a translation in z we get the analogues of (4.2) and (4.3):

$$(r-s)\tilde{B}(r,s;z) = -\tilde{B}(r+1,s;z+1) - \tilde{B}(r-1,s;z+1) + \tilde{B}(r,s+1;z+1) + \tilde{B}(r,s-1;z+1), \tag{4.21}$$

and

$$(r^2 - s^2)\tilde{B}(r, s; z) = -\tilde{B}(r + 1, s; z + 1) - \tilde{B}(r - 1, s; z + 1) + \tilde{B}(r, s + 1; z + 1) + \tilde{B}(r, s - 1; z + 1), \tag{4.22}$$

respectively. The only difference in form between eqs. (4.2) and (4.3) and eqs. (4.21) and (4.22) is that $j - 1$ transforms into $z + 1$. Separation of variables works as before, with $-z$ instead of j, but with a new twist. To see this, consider the following hypothesis

$$\tilde{B}(r, s; c) = f(r + s + z)g(-r + s - z)h(r + s - z)t(r - s - z)u(z) \tag{4.23}$$

and new variables $\bar{a} = r + s + z$, $b = -r + s - z$, $c = r + s - z$, $d = r - s - z$. Notice that $\bar{a}$ has $+z$ instead of $-z$. Variables separate and we can reproduce the previous solutions using the Γ function instead of factorials. For example, in the case of the Quantum Pendulum the simplest case $G^1_{0,0,0}$ corresponds to

$$\tilde{B}(r, s; z) = \frac{(-1)^{\frac{r+s-z}{2}}\Gamma(\frac{r+s+z}{2})}{\Gamma(1 + \frac{-r+s-z}{2})\Gamma(1 + \frac{r+s-z}{2})\Gamma(1 + \frac{r-s-z}{2})}. \tag{4.24}$$

Notice that instead of having four factorials in the denominator we have three Γ functions in the denominator with $-z$ and a Γ function with $+z$ in the numerator. This is as it must be, the inverse Mellin transform should be seen as a sum over the residues of

$$\tilde{B}(r, s; z)c^{-z} \tag{4.25}$$

and then the residues of Γ at the negative integers give us the extra factorial in the denominator. Notice also that it is best to see the inverse Mellin transform as a sum over residues and not as an integral over a vertical line as in its formal definition (A.16), because a factor of the form $(-1)^z = e^{\pm i\pi z}$ grows exponentially in one of the vertical directions.

Given the new necessary asymmetry between one of the variables and the rest of the variables used in the separation of variables, new solutions appear with two Γ functions with $+z$ in the numerator. This corresponds to the existence of double poles of the Mellin transform. When we now do the inverse Mellin transform of these new solutions the derivative of the Γ function makes its appearance and the new solutions are no longer hypergeometric functions but involve also Harmonic numbers. Due to lack of space we will say no more about this topic for the time being.

4.2 Direct approaches vs Wigner transforms of Helmholtz solutions

Here, one wishes to compare the integral operators refered to in section 2.5.2 and studied in section 3.5 with the operators obtained in previous section. To do so, the series expansions in powers of the coupling constant $c = -\lambda I/\hbar^2$ of the matrix elements $\langle r|\hat{A}|s\rangle$ will be computed.

4.2.1 Simplest cartesian

Starting with the integral operator studied in 3.5.1, whose matrix elements in the angular variables read

$$\langle\theta_1|\hat{A}|\theta_2\rangle = \cos\left[\Omega\cos\left(\frac{\theta_1}{2}\right)\cos\left(\frac{\theta_2}{2}\right)\right], \tag{4.26}$$

one finds, accounting for (3.140) and the fact that $\Omega^2 = 16c$:

$$\langle\theta_1|\hat{A}|\theta_2\rangle = \sum_{j=0}^{\infty}\frac{\Omega^{2j}(-1)^j}{(2j)!}\left[\cos\left(\frac{\theta_1}{2}\right)\right]^{2j}\left[\cos\left(\frac{\theta_2}{2}\right)\right]^{2j} = \sum_{j,l,k=0}^{\infty}\frac{(-c)^j(2j)!}{l!(2j-l)!k!(2j-k)!}e^{i(j-l)\theta_1}e^{i(j-k)\theta_2}. \tag{4.27}$$

Defining $r = j - l$ and $-s = j - k$, and recalling (2.97) and (2.99),

$$\langle r|\hat{A}|s\rangle = 2\pi\sum_{j=0}^{\infty}\frac{(-1)^j(2j)!}{(j-r)!(j+r)!(j+s)(j-s)!}c^j. \tag{4.28}$$

It is readily apparent that this solution is not one of those retrieved in section 4.1 and, although it should be possible to derive (4.28) by solving (4.3) using separation of variables, it is far from obvious how to proceed with it without already knowing the outcome of the exercise.

4.2.2 Polar

As observed in section 3.5.2 the Wigner transforms of the solutions in polar coordinates of the Helmholtz equation mentioned in section 2.5.2 are linear combinations of elements of the first family of solutions obtained directly in section 3.2.2. In section 3.4, the latter solutions were seen to be a subfamily of the first family in section 3.3.2. Therefore, the matrix elements of the corresponding operators in the angular momentum basis are given in section 4.1.2 by a subfamily of (4.16) with $d_1 = \pm 2p$ and $d_2 = 0$. Consequently, the matrix elements of the integral operators defined by the solutions in polar coordinates of the Helmholtz eq. are linear combinations of the expressions in section 4.1.2.

If, on the other hand, one tries to compute the matrix elements in the angular momentum basis directly from the integral kernel, it will be found that the task is highly nontrivial, as we now proceed to illustrate.

Following a similar path as in the previous section, the matrix elements in the angle representation for the simplest solution with $p = 0$ are those given in (B.14), which can now be rewritten as

$$\langle\theta_1|\hat{A}|\theta_2\rangle = \sum_{j=0}^{\infty}\frac{\Omega^{2j}(-1)^j}{8^j j!j!}[\cos(\theta_1)+\cos(\theta_2)]^j = \sum_{j=0}^{\infty}\sum_{l=0}^{j}\sum_{p=0}^{l}\sum_{q=0}^{j-l}\frac{(-c)^j}{j!p!(l-p)!q!(j-l-q)!} \times e^{i(l-2p)\theta_1}e^{i(j-l-2q)\theta_2} \tag{4.29}$$

and, changing once more to r and s,

$$\langle r|\hat{A}|s\rangle = 2\pi \sum_{\substack{j \text{ same parity} \\ \text{as } r+s}} \sum_{\substack{l \text{ same parity} \\ \text{as } r}} \frac{(-1)^j}{j!\left(\frac{l-r}{2}\right)!\left(\frac{l+r}{2}\right)!\left(\frac{j-l-s}{2}\right)!\left(\frac{j-l+s}{2}\right)!} c^j. \tag{4.30}$$

In view of comparing with (4.16), one still has to sum over l in (4.30), which, for example, for matrix elements with even indices, becomes

$$\begin{aligned}\langle 2r|\hat{A}|2s\rangle =& 2\pi \sum_j \frac{c^{2j}}{(2j)!} \sum_l \frac{1}{(l-r)!(l+r)!(j-l-s)!(j-l+s)!} \\ =& 2\pi \sum_j \frac{c^{2j}}{(2j)!} \frac{1}{(j-r-s)!(j+r+s)!} \sum_l \binom{j-r-s}{l-r}\binom{j+r+s}{l+r}\end{aligned} \tag{4.31}$$

Making $k = l - r$ and using the identity $\binom{m}{n} = \binom{m}{m-n}$,

$$\langle 2r|\hat{A}|2s\rangle = 2\pi \sum_j \frac{c^{2j}}{(2j)!} \frac{1}{(j-r-s)!(j+r+s)!} \sum_k \binom{j-r-s}{k}\binom{j+r+s}{j-r+s-k}, \tag{4.32}$$

or, making use of the combinatorial identity (see (3.4) in [25])

$$\sum_{k=0}^{n} \binom{n}{k}\binom{x+y-n}{x-k} = \binom{x+y}{x}, \tag{4.33}$$

with $x = j - r + s$, $n = j - r - s$ and $y = j + r - s$,

$$\begin{aligned}\langle 2r|\hat{A}|2s\rangle =& 2\pi \sum_j \frac{c^{2j}}{(2j)!} \frac{1}{(j-r-s)!(j+r+s)!} \binom{2j}{j-r+s} \\ =& 2\pi \sum_j \frac{1}{(j+r+s)!(j-r-s)!(j+r-s)!(j-r+s)!} c^{2j}\end{aligned} \tag{4.34}$$

which is the same, modulo the 2π factor, as (4.16), with $j_0 = d_1 = d_2 = 0$, as it should.

This was the result for the simplest solution with $p = 0$, when $p > 0$ the result seems even more difficult to achieve via the direct route.

4.2.3 Helmholtz solutions in elliptic coordinates

In section 2.5 the link between matrix elements of integral operators and Fourier coefficients of their integral kernels was referred. Moreover, the connection between integral kernels of stationary operators and the solutions to the Helmholtz 2d equation in modified elliptic coordinates was also mentioned. One can now revert our solutions in modified elliptic coordinates back to normal elliptic coordinates by identifying $\xi = i\theta_1/2$ and $\eta = \theta_2/2$, that is, $x = \cosh(\xi)\cos(\eta)$ and $y = \sinh(\xi)\sin(\eta)$. The products of complex exponentials in θ_1 and θ_2 become products of real and complex exponentials in ξ and η and products of cosines or sines become products of hyperbolic cosines and cosines or hyperbolic sines and sines. This means we can write the solutions $u(x, y) = \cos(\Omega x)$ and $u(r, \phi) = J_{2p}(\Omega r)\cos(2p\phi)$ in elliptic coordinates as sums of products of the form $\cosh(r\xi)\cos(s\eta)$, with r and s even, in a closed form; and the solutions $u(r,\phi) = J_{2p}(\Omega r)\sin(2p\phi)$ in elliptic coordinates as sums of products of the form $\sinh(r\xi)\sin(s\eta)$ with r and s even, also in a closed form.

The writing of the polar solutions in elliptic coordinates is the more relevant since they provide a basis for the space of functions generated by products of modified Mathieu times Mathieu functions of even index, that is, $Ce_{2n}(\xi)ce_{2n}(\eta)$ and $Se_{2n}(\xi)se_{2n}(\eta)$. What remains to be done is to give closed forms for the products of Mathieu functions themselves. In the next section we discuss several approaches to this problem.

4.3 Links to stationary pure states and Mathieu functions

4.3.1 Generalities on the Simplified Hindered Rotator

In section 2.5.1 it was referred that the matrix elements of pure states have a product form $\langle r|\hat{\rho}|s\rangle = C_r C_s^*$. Also, in section 2.1.3 we derived the wave function solutions to the SHR model. This was followed in section 2.3.1 by the computation of their Wigner transforms (2.49). After that, in section 3.2.1, we saw that the latter could be obtained directly by solving the stationarity equation. Following that, we computed the Fourier coefficients of these solutions in section 3.4.1. From the correspondence between Fourier coefficients and matrix elements we can infer that the solutions in (4.10) with $j_0 = d_2 = 0$ and $d_1 = -2d$ are the stationary pure states associated to energies $E = \hbar\omega d$.

It is natural to ask if these matrix elements could have been obtained in a more direct way. This is indeed the case as will be seen. If one starts with the Fourier coefficients of the wave functions (2.18) which are given by Bessel functions $J_{r-d}(-2c)$ and then one uses the formula for the product of Bessel functions (A.28) to get:

$$\langle r|\hat{\rho}_d|s\rangle = \langle r|\psi_d\rangle\langle\psi_d|s\rangle = J_{r-d}(-2c)J_{s-d}(-2c) = \sum_{k=0}^{\infty} \frac{(-1)^k (r+s-2d+2k)!(-c)^{r+s-2d+2k}}{(r+s-2d+k)!(r-d+k)!(s-d+k)!k!}. \quad (4.35)$$

Next, consider a member of the third family $\hat{A}^3_{j_0,d_1,d_2}$ specified by (4.10), with $j_0 = d_2 = 0$ and $d_1 = -2d$,

$$\langle r|\hat{A}^3_{0,-2d,0}|s\rangle = \sum_{\substack{j \text{ same} \\ \text{parity as} \\ r+s-2d}} \frac{(-1)^{\frac{j+r+s}{2}} j!}{(\frac{j+r+s-2d}{2})!(\frac{j-r-s+2d}{2})!(\frac{j+r-s}{2})!(\frac{j-r+s}{2})!} c^j, \quad (4.36)$$

and change variables according to $j = r+s-2d+2k$, so that

$$\langle r|\hat{A}^3_{0,-2d,0}|s\rangle = \sum_{k=-\infty}^{\infty} \frac{(-1)^{r+s-d+k}(r+s-2d+2k)!c^{r+s-2d+2k}}{(r+s-2d+k)!k!(r-d+k)!(s-d+k)!}. \quad (4.37)$$

Remembering that $1/k! = 0$ for negative k, we see that this last expression is equal to (4.35) times a constant multiplier $(-1)^d$, telling us in particular that the subfamily of operators $\hat{\rho}_d = \hat{A}^3_{0,-2d,0}$ does correspond to pure states since its matrix elements have a product form $J_{r-d}(-2c)J_{s-d}(-2c)$. Trying to prove that $\hat{A}^3_{0,-2d,0}$ is a pure state by proving that the square of the operator satisfies

$$\left(\hat{A}^3_{0,-2d,0}\right)^2 = \hat{A}^3_{0,-2d,0}, \tag{4.38}$$

seems a lot harder, although not impossible.

4.3.2 Mathieu functions through linear conditions

If we could write products of Mathieu functions $ce_{2n}(\theta_1/2)ce_{2n}(\theta_2/2)$ or $se_{2n}(\theta_1/2)se_{2n}(\theta_2/2)$ in a closed form we would then get a closed form for the Mathieu functions themselves by simply making $\theta_1 = \theta_2$ and taking a square root. The sign would have to be guessed from the continuity of the derivative. In the previous chapter and in the beguinning of this one, five families of solutions of the stationarity equations were found and one would like to know if any of these is proportional to a pure state. The ones that correspond to solutions of the Helmholtz equation that are separated in a coordinate system different from modified elliptic coordinates can be safely considered not to be pure states. What about the other solutions? It ends up being the case as we shall see that they are also not pure states, but the question remains, are there simple linear combinations of these solutions that are pure states? Let us try to obtain information on this problem.

Boundary conditions

Perturbation theory for the Mathieu functions was reviewed in section 2.2.2. The first Taylor coefficients different from zero of the Mathieu coefficients are known and do not depend on the normalization, so if we consider products of Mathieu coefficients, their first Taylor coefficients different from zero are simply the product of the Taylor coefficients of the corresponding individual Mathieu coefficients and also do not depend on the normalization. Making use of the notation $F^{(2n)}(r,s,j)$ for the power-series coefficients of the matrix elements $\langle r|ce_{2n}\rangle\langle ce_{2n}|s\rangle$, that is,

$$\frac{1}{2\pi}\langle r|ce_{2n}\rangle\langle ce_{2n}|s\rangle = \sum_{j\in\mathbb{Z}} F^{(2n)}(r,s,j)c^j, \tag{4.39}$$

and using (2.39) we get the following boundary condition for $F^{(2n)}(r,s,j)$:

$$F^{(2n)}(r,s,r+s-2n) = \frac{1}{4}(-1)^{r+s-2n}\frac{(2n)!(2n)!}{(r-n)!(r+n)!(s-n)!(s+n)!}, \tag{4.40}$$

whereas

$$F^{(2n)}(r,s,j) = 0 \tag{4.41}$$

for $j < r+s-2n$, when $r,s \geq n > 0$.

Closed forms of stationary observables were presented in 4.1.2 for four different families, hence, to see if any of them corresponds to pure states, we should compare the first non-zero coefficients of their Taylor series in powers of the parameter $c = q/4$ with the first non-zero Taylor coefficients of products of

Mathieu coefficients. More precisely, using the notation $G^i_{j_0,d_1,d_2}(r,s,j)$ for the power-series coefficients of the matrix elements of the operators $\hat{A}^i_{j_0,d_1,d_2} := 2\pi c^{-j_0}\hat{A}_{d_1,d_2}$ (with $i = 1, 2, 3, 4$) given in section 4.1.2,

$$\frac{1}{2\pi}\langle r|\hat{A}^i_{j_0,d_1,d_2}|s\rangle = \sum_{j=-\infty}^{\infty} G^i_{j_0,d_1,d_2}(r,s,j)c^j \tag{4.42}$$

we can try to see if any of the $G^i_{j_0,d_1,d_2}(r,s,j)$ satisfies the boundary condition (4.40).

Now, from (4.18), with $j_0 = 2n$, $d_1 = 0$, and $d_2 = 2n$, we have

$$G^3_{2n,0,2n}(r,s,r+s-2n) = \frac{(-1)^{r+s}(r+s)!}{(r+s)!0!(r+n)!(r-n)!(s+n)!(s-n)!} = \frac{(-1)^{r+s}}{(r+n)!(r-n)!(s+n)!(s-n)!}, \tag{4.43}$$

which verifies the boundary condition (4.40) with $(2n)!^2 G^3_{2n,0,2n}/4$, this being true for the case $n > 0$. For the case $n = 0$, the factor $1/4$ doesn't appear and we satisfy the boundary condition with $G^3_{0,0,0}$. So, it might seem that we have finally solved the problem of finding closed forms for the Mathieu coefficients. Unfortunately, such is not the case: what happens is that the above calculations were done for the case where r and s are both greater than 0. If, for example, $s < 0$ and $r > -s \geq n > 0$, we then substitute throughout s by $-s$ and the boundary condition is now at points $(r, s, r-s-2n)$, this new boundary condition being now satisfied by $(2n)!^2 G^2_{2n,2n,0}/4$ and, likewise, by $G^2_{0,0,0}$ if $n = 0$.

However, this should not yet come as a showstopper, because linear combinations of stationary solutions are again stationary, so we may try to find linear combinations that satisfy the boundary conditions. For example, given that $G^3_{2n,0,2n}(r,s,r-s-2n) = 0$ for $n > 0$, since the argument of the last factorial in the denominator of (4.43) becomes negative, and similarly that $G^2_{2n,2n,0}(r,s,r+s-2n) = 0$, we might try the linear combination $(2n)!^2(G^2_{2n,2n,0} + G^3_{2n,0,2n})/4$ for $n > 0$. What goes wrong with the latter becomes apparent when we try to apply it to the case $n > r, s \geq 0$: we now must use (2.35), instead of (2.34), and the boundary conditions are now given at points $(r, s, 2n-r-s)$. It is then easy to check that, for instance, when $n = 1$ and $r, s = 0$, we have $F^{(2)}(0,0,2) = 1$, $G^2_{2,2,0}(0,0,2) = 4!/(3!1!3!1!2!2!) = 1/6$, and $G^3_{2,0,2}(0,0,2) = 4!/(2!2!3!1!3!1!) = 1/6$, so the above linear combination fails in this case. The true problem is that the expressions (2.34) and (2.35) are not symmetric with respect to the role of r, so it seems we should involve the other two families $G^1_{j_0,d_1,d_2}$ and $G^4_{j_0,d_1,d_2}$, but it is not obvious how to do it.

In the case $n = 0$, a linear combination that works for all cases is $G^2_{0,0,0} + G^3_{0,0,0} - G^1_{0,0,0}$ and so, again, it would seem that we have solved the problem of finding the Mathieu coefficients of ce_0. Yet, now we face an even deeper problem, its having never been proven that the boundary conditions are sufficient to determine the behavior of $F^{(2n)}(r,s,j)$ in the whole of $\mathbb{Z}^3$, and such is indeed not the case. In fact, $G^4_{0,0,0}$ also satisfies the boundary conditions.

In the particular case of ce_0, the second non-zero Taylor coefficients of the ratio of Mathieu coefficients $A^{(0)}_{2r}/A^{(0)}_0$ are known. If one tries to compare the values of $F^{(0)}$ determined by these Taylor coefficients with the ones given by the linear combination $G^2_{0,0,0} + G^3_{0,0,0} - G^1_{0,0,0}$, a mismatch will be found, implying that new stationary operators operators must be taken into consideration. In the case of $G^4_{0,0,0}$ there also does not appear to be any possible normalization of ce_0 compatible with the values of

$G^4_{0,0,0}(r, s, r + s + 2)$.

Linear combinations

We know that the first discrete family with $d_2 = 0$ is a basis of the space of solutions. From section 3.5.2, especially (3.165), we know that the operators given by solutions of the Helmholtz equation of the form $u(r, \phi) = J_{2p}(\Omega r)\cos(2p\phi)$ correspond to the linear combinations of operators

$$\frac{1}{2}\left(\hat{A}^1_{p,-2p,0} + \hat{A}^1_{-p,2p,0}\right). \tag{4.44}$$

Since these solutions of the Helmholtz equation generate the space of functions generated by the products of even Mathieu functions $ce_{2n}(\theta_1/2)ce_{2n}(\theta_2/2)$ we have that it is necessarily the case that for each pure state there are coefficients α^n_d, with $\alpha^n_{-d} = \alpha^n_d$, such that

$$\frac{1}{2\pi}|ce_{2n}\rangle\langle ce_{2n}| = \sum_{d=-\infty}^{\infty} \alpha^n_d \hat{A}^1_{-d,2d,0}. \tag{4.45}$$

If we now expand these coefficients into powers of the coupling constant

$$\alpha^n_d = \sum_k \alpha^n_{d,k} c^k, \tag{4.46}$$

we obtain the following decomposition

$$F^{(2n)} = \sum_{d=-\infty}^{\infty} \sum_k \alpha^n_{d,k}\, G^1_{-k-d,2d,0}. \tag{4.47}$$

A closed form for the Mathieu functions would be achieved if one could obtain a closed form for the coefficients $\alpha^n_{d,k}$. For this we need linear equations. Infinitely many of them, and, preferably, each linear equation should have only a finite number of terms.

The boundary conditions of the previous section provide a first set of equations. Let us look at the case $n = 0$. Here the boundary equations read

$$\sum_{d,k} \alpha^0_{d,k}\, G^1_{-k-d,2d,0}(r, s, |r| + |s|) = \frac{(-1)^{r+s}}{|r|!|r|!|s|!|s|!}, \qquad \forall r, s \in \mathbb{Z} \tag{4.48}$$

If r and s are both non-negative then, supposing that $k \geq 0$, the only terms that survive are those with k of the same parity as d, d nonnegative, $k \leq d$, and $d \leq \min\{r, s\}$, so that we have only finitely many terms in each equation. One now recursively tries to solve this infinite set of equation by increasing r and s, starting with $r = s = 0$. Dropping the superscript 0, one then finds that $\alpha_{0,0} = 1$, $\alpha_{1,1} = 1$ and $\alpha_{2,0} = 0$. Speculating that $\alpha_{d,k} = 0$ when $k < d$, one can try to find an expression for $\alpha_{d,d}$ that solves (4.48) in all cases where r and s are non-negative. This can indeed be achieved. An expression that works is

$$\alpha_{d,d} = \frac{1}{d!d!}. \tag{4.49}$$

This can be verified with the help of (4.33). We can now ask the question: what is the result of summing the right hand side of (4.47) with this expression for the coefficients $\alpha_{d,k}$? Using the combinatorial identity (see (3.20) in [25])

$$\sum_{k=0}^{n}\binom{n}{k}\binom{x}{k+r}=\binom{n+x}{n+r} \tag{4.50}$$

one arrives at

$$\sum_{d=0}^{\infty}\alpha_{d,d}G^{1}_{-2d,2d,0}=G^{3}_{0,0,0}. \tag{4.51}$$

This is quite interesting since we had already seen that $G^3_{0,0,0}$ satisfies the boundary conditions when r and s are non-negative. When r and s have different signs the terms that survive in (4.48) are those with d negative or zero. The situation is entirely symmetric and one gets that $\alpha_{d,d}=1/(|d|!|d|!)$ and $\alpha_{d,k}=0$ when $k<|d|$, works. Summing in d non-positive

$$\sum_{d=-\infty}^{0}\alpha_{d,d}G^{1}_{-2d,2d,0}=G^{2}_{0,0,0}, \tag{4.52}$$

so that

$$\sum_{d=-\infty}^{\infty}\alpha_{d,d}G^{1}_{-2d,2d,0}=G^{3}_{0,0,0}+G^{2}_{0,0,0}-G^{1}_{0,0,0}. \tag{4.53}$$

We had already seen that this linear combination satisfies the boundary conditions, so it is natural to conjecture that indeed the above expressions for $\alpha_{d,k}$ for $k\le|d|$ are the right ones. I was able to determine that $\alpha_{4,0}=0$ as expected.

The above was done for the case $n=0$, the vacuum state. When $n\ge1$ things get a little more complicated as already explained in the previous section. In the case where $r,s\ge n$, if we suppose $k\ge -n$ we will have conditions for $d\ge n$ and k between $-n$ and $d-2n$. Again supposing $\alpha^n_{d,k}=0$ if $k<d-2n$ we have a solution with

$$\alpha^{n}_{d,d-2n}=\frac{(2n)!(2n)!}{4(d-n)!(d+n)!}. \tag{4.54}$$

Summing with the help of (4.50) we get

$$\sum_{d=n}^{\infty}\alpha^{n}_{d,d-2n}G^{1}_{2n-2d,2d,0}=\frac{(2n)!(2n)!}{4}G^{3}_{2n,0,2n}, \tag{4.55}$$

which we already knew satisfied the boundary conditions when $r,s\ge n$. There certainly seems to be a pattern here.

Although the boundary conditions provide interesting information one would like to compute all $\alpha^n_{d,k}$, not just the coefficients that get the first non-zero Taylor coefficients right. We need a new set of equations. A possibility is related to the issue of normalization. The trace of any density operator must be equal to one. This means that the trace has no dependence on the coupling constant. Translating this into our language we obtain

$$\sum_{d,k,r} \alpha^n_{d,k} G^1_{-k-d,2d,0}(r,r,j) = 0, \qquad \forall j \geq 1. \tag{4.56}$$

The number of terms in each equation is effectively finite, but, unfortunately the equations are not enough to determine all the coefficients, since we are just asking for a stationary operator of trace 1. Nevertheless it may be the case that one can use these equations to eventually conjecture a closed form for the coefficients. One could then try to prove that the coefficients are indeed correct by proving that $\hat{\rho}^2 = \hat{\rho}$. This leads us to our final theme.

4.3.3 Mathieu functions - embracing the non-linearity

Direct factorization

In this approach, we try to do linear combinations of stationary observables in order to obtain an operator whose matrix elements can be factored in the form $C_r C_s^*$, which factorisation was achieved using the formula for the product of Bessel functions (A.28) in the SHR case. The proof of this formula uses the so-called Vandermonde convolution [26]

$$\sum_{j=0}^{n} \binom{a}{j}\binom{b}{n-j} = \binom{a+b}{n}, \tag{4.57}$$

and one can try to use the vast field of combinatorial identities to get something similar for the QP problem. However, the families of solutions in 4.1.2 involve more factorials than the ones in 4.1.1, implying, therefore, that the kind of combinatorial identities we are trying to work with involve sums of products of three or more binomial coefficients and, *hélas*, there is a much smaller body of knowledge in this case. This is not the main objection to this path. A stronger objection is that it may happen that products of Mathieu coefficients are hypergeometric functions of the coupling constant without this being the case for the Mathieu coefficients themselves. Square roots of hypergeometric functions need not be hypergeometric. But the main objection is that it is difficult to concoct a systematic approach to achieve the required factorization.

Equations for pure states

From the evolution equations (2.60) and (2.61) for the SHR and QP models, respectively, defining the Fourier coefficients as functions of the coupling constant by $f(r;c) := \langle r|\psi\rangle$ and supposing they are real, we get the non-linear functional equations

$$(r-s)f(r;c)f(s;c) = c\Big(f(r;c)f(s+1;c)+f(r;c)f(s-1;c)-f(r+1;c)f(s;c)-f(r-1;c)f(s;c)\Big) \tag{4.58}$$

and

$$(r^2-s^2)f(r;c)f(s;c) = c\Big(f(r;c)f(s+1;c)+f(r;c)f(s-1;c)-f(r+1;c)f(s;c)-f(r-1;c)f(s;c)\Big). \quad (4.59)$$

These equations are equivalent to the time-independent Schrödinger equations (2.5) and (2.6) for the Fourier coefficients. The latter can be obtained by simply separating variables.

We have seen that the Wigner function and consequently the density operator representation are privileged settings to obtain closed forms for solutions. So perhaps it is better to leave the equations in product form instead of separating variables. One then tries to reproduce the solutions of the SHR model that we already know of and, possibly, only minor changes will be necessary to get the solutions to the QP model. Trying to do this one must take into consideration the main difference between these two models, the fact that eigenvalues do not change with the coupling constant in the SHR model. For example, if we do a Mellin transform of the dependence of the coefficients on the coupling constant we get

$$\begin{aligned}(r-s)\int_L \tilde{f}(r;w)\tilde{f}(s;z-w)dw &= \int_{L_1} \tilde{f}(r;w_1)\tilde{f}(s+1;z+1-w_1)dw_1 \\ &+ \int_{L_2} \tilde{f}(r;w_2)\tilde{f}(s-1;z+1-w_2)dw_2 - \int_{L_3} \tilde{f}(r+1;w_3)\tilde{f}(s;z+1-w_3)dw_3 \\ &- \int_{L_4} \tilde{f}(r-1;w_4)\tilde{f}(s;z+1-w_4)dw_4\end{aligned} \quad (4.60)$$

for the SHR model and the same expression with r^2-s^2 instead of $r-s$ for the QP model. The contours L_i must be appropriately chosen. If we now take $w_1=w$, $w_2=w$, $w_3=w+1$ and $w_4=w+1$ and put everything in the same integral we could think on demanding that the integrand function is zero, that is,

$$\begin{aligned}(r-s)\tilde{f}(r;w)\tilde{f}(s;z-w) - \tilde{f}(r;w)[\tilde{f}(s+1;z+1-w) + \tilde{f}(s-1;z+1-w)] \\ + [\tilde{f}(r+1;w+1) + \tilde{f}(r-1;w+1)]\tilde{f}(s;z-w) = 0.\end{aligned} \quad (4.61)$$

This can indeed be achieved if, for example, the functions $\tilde{f}(n;v)$ satisfy

$$n\tilde{f}(n;v) = -\tilde{f}(n+1;v+1) - \tilde{f}(n-1;v+1). \quad (4.62)$$

But this is simply the Mellin transform of the time-independent Schrödinger equation (2.5) with eigenvalue $d=0$. This does not work if the eigenvalue depends on the coupling constant. In that case one must also take a Mellin transform of the eigenvalue and consider Mellin convolutions between Fourier coefficients and eigenvalues. So it seems that the stronger condition (4.61), with r^2-s^2 instead of $r-s$, that the integrand is zero is too strong in the case of the Quantum Pendulum.

Nevertheless, one can still try to solve (4.60) without supposing that the integrand is zero. In this case one must sum over residues. This is not complicated given the fact that meromorphic functions are determined by their zeros and poles in the form of an infinite product and so we can suppose that $\tilde{f}(r;z)$ is of the form a Γ function times an entire function or a function with poles on the right side of the plane. We can do even more and suppose $\tilde{f}(r;z)$ is given by an infinite product with zeros and poles on the integers only. But, unfortunately there doesn't seem to be a natural way to extend the process from which we reproduce the solutions of the SHR model we already know of to the case of the QP model. Here the change from $r-s$ to r^2-s^2, if achievable, seems to require the use of a computer algebra program. Ultimately, one must take into consideration what was said in the previous section, it may be that Mathieu coefficients are not hypergeometric functions of the coupling constant. In this case, their Mellin transforms need not have nice infinite product representations.

Product formula

If Mathieu coefficients are not hypergeometric functions of the coupling constant but their products are, then one should work directly with the products, that is, matrix elements of operators or, equivalently, Fourier coefficients of the Wigner function. Let us think in terms of operators. Then the property of being a pure state is equivalent to $\hat{\rho}^2 = \hat{\rho}$ which can written as

$$\sum_{l=-\infty}^{\infty} \langle r|\hat{\rho}|l\rangle\langle l|\hat{\rho}|s\rangle = \langle r|\hat{\rho}|s\rangle, \qquad \forall r,s \in \mathbb{Z}. \tag{4.63}$$

There are two ways to use this formula. One can try to use it in parallel with the formula for stationarity

$$(r-s)\langle r|\hat{\rho}|s\rangle = c\big(\langle r|\hat{\rho}|s+1\rangle + \langle r|\hat{\rho}|s-1\rangle - \langle r+1|\hat{\rho}|s\rangle - \langle r-1|\hat{\rho}|s\rangle\big) \tag{4.64}$$

to reproduce the solutions of the SHR model as power series in the coupling constant and then try to adapt the procedure to the QP model. The second way is to start from a basis of stationary solutions and just use (4.63) to produce a linear combination that is a stationary pure state. In both cases one must deal with the non-linearity of (4.63) and the fact that the number of factorials in the terms that appear doubles. So one must also take into consideration that there are not that many combinatorial identities that involve so many factorials (at least eight of them) with the same parameter. We had already alluded to this problem at the end of 4.3.1 when we mentioned that even verifying that $\hat{\rho}_d$ was a pure state from the product formula was likely to be non-trivial. Nevertheless, I think it is an exercise worth undertaking, some information will certainly be obtained.

Chapter 5

Conclusions

5.1 Achievements

In this thesis two models were studied, the first a solvable model as a simplification of the main model of interest, the Quantum Pendulum. Several families of solutions to the stationarity equations for these models were obtained, both in the Wigner function representation and in the Density Operator representation. In both cases the solutions were given as power series in the coupling constant.

A new simplified derivation of the evolution equations was performed using the Density Operator representation. Moreover, the integral form of the Moyal bracket was also studied and used to derive the evolution equations.

Finally, connections to the Helmholtz equation in two dimensions in elliptic coordinates and to Mathieu functions were discussed.

5.2 Future Work

The most immediate work to be done is to verify that the stationary pure state solutions of the Simplified Hindered Rotator satisfy the property $\hat{\rho}^2 = \hat{\rho}$ or, equivalently, $w\bigstar w = w$. It may be that this is yet again a field where the Wigner function provides a simpler route to success. If this is achieved the next step is to try to adapt the proof to the case of the Quantum Pendulum, probably using the simplest basis of stationary solutions.

Another direction for future work is to start from the integral form of the equation $w\bigstar w = w$ and, using the stationarity equation, try to develop an integral form for the Taylor coefficients of the solution in the spirit of Feynman diagramms.

Bibliography

[1] E. Mathieu. Mémoire sur le mouvement vibratoire d'une membrane de forme elliptique. *Journal de Mathématiques Pures et Appliquées*, 13:137–203, 1868.

[2] J. P. Bizarro. *Phys. Rev. A*, 49:3255, 1994. *errata*, 71:069901, 2005.

[3] E. Wigner. On the quantum correction for thermodynamic equilibrium. *Phys. Rev.*, 40(5):749–759, 1932.

[4] L. Cohen. *Time-Frequency Analysis*. Prentice-Hall, 1995.

[5] R. F. O'Connell and E. P. Wigner. *Phys. Lett.*, 83A:145, 1981.

[6] M. Hillery, R. F. O'Connell, M. O. Scully, and E. P. Wigner. *Phys. Rep.*, 106:121, 1984.

[7] M. V. Berry. *Phil. Trans. R. Soc. Lond. A*, 287:237, 1977.

[8] N. Mukunda. *Am. J. Phys.*, 47:182, 1979.

[9] G. P. Berman and A. R. Kolovsky. *Physica*, 17D:183, 1985.

[10] J. E. Moyal and M. S. Bartlett. Quantum mechanics as a statistical theory. *Proc. Camb. Phil. Soc.*, 45:99, 1949.

[11] H. J. Groenewold. On the principles of elementary quantum mechanics. *Physica*, 12(5):405–460, 1946.

[12] G. Baker. Formulation of quantum mechanics based on the quasi-probability distribution induced on phase space. *Phys. Rev.*, 109:2198–2206, 1958.

[13] D. S. K. Chan. In *Proceedings of the IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP '82)*, page 1333, Piscataway, NJ, 1982. IEEE.

[14] J. P. S. Bizarro and A. C. A. Figueiredo. *Nucl. Fusion*, 46:645, 2006.

[15] E. U. Condon. The physical pendulum in quantum mechanics. *Phys. Rev.*, 31:891–894, May 1928.

[16] N. W. McLachlan. *Theory and Application of Mathieu functions*. Oxford, Clarendon Press, 1951.

[17] G. Blanch. Mathieu functions. In M. Abramowitz and I. A. Stegun, editors, *Handbook of Mathematical Functions*, National Bureau of Standards Applied Mathematics Series 55, pages 721–750, Washington, D.C., 1972. U.S. Government Printing Office.

[18] G. Wolf. Mathieu functions and hill's equation. In F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark, editors, *NIST Handbook of Mathematical Functions*, pages 651–682, New York, 2010. Cambridge University Press.

[19] T. Pradhan and A. V. Khare. *Am. J. Phys.*, 41:59, 1973.

[20] R. Aldrovandi and P. L. Ferreira. *Am. J. Phys.*, 48:660, 1980.

[21] F. Peyrin and R. Prost. *IEEE Trans. Acoust. Speech Signal Process*, ASSP-34:858, 1986.

[22] T. A. C. M. Claasen and W. F. G. Mecklenbräuker. *Philips J. Res.*, 35:217, 1980.

[23] W. Miller. *Symmetry and Separation of Variables*, volume 4 of *Encyclopedia of Mathematics and its Applications*. Addison-Wesley, Reading, MA, 1977.

[24] W. G. Kelley and A. C. Peterson. *Difference Equations: An Introduction with Applications*. Academic Press, San Diego, CA, 2nd edition, 2001.

[25] H. W. Gould. *Combinatorial Identities*. Academic Press, Morgantown, WV, revised edition, 1972.

[26] G. N. Watson. *A Treatise on the Theory of Bessel Functions*. Cambridge University Press, Cambridge, 2nd edition, 1966.

[27] M. Petkovšek, H. Wilf, and D. Zeilberger. *A=B*. A K Peters/CRC Press, 1996.

[28] F. W. J. Olver. Bessel functions of integer order. In M. Abramowitz and I. A. Stegun, editors, *Handbook of Mathematical Functions*, National Bureau of Standards Applied Mathematics Series 55, pages 355–434, Washington, D.C., 1972. U.S. Government Printing Office.

[29] F. W. J. Olver and L. C. Maximon. Bessel functions. In F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark, editors, *NIST Handbook of Mathematical Functions*, pages 215–286, New York, 2010. Cambridge University Press.

Appendix A

Generalized Hypergeometric functions

All the solutions of the stationarity equations will be given in terms of Generalized Hypergeometric Functions or *Hypergeometric Functions* for short. Intuitively, a function is hypergeometric if it can be written as a power series where the Taylor coefficients are combinations of factorials. More precisely, if t_k is the k-th Taylor coefficient then t_{k+1}/t_k is a rational function of k, that is,

$$\frac{t_{k+1}}{t_k} = \frac{p(k)}{q(k)}, \tag{A.1}$$

where $p(z)$ and $q(z)$ are polynomials. This class of functions includes most of the special functions usually taught in a Physics degree like exponentials, trigonometric, Bessel, Hermite, etc. Unfortunately, all the conventions used to represent these functions are bad for our purposes, so I chose to leave most solutions in power series form, the exception being Bessel functions and functions whose terms have few factorials. Paradoxically, from the typesetting point of view it is more concise to write the power series then it is to use the standard notations. If one wants to implement the associated functions in a software package capable of symbolic computations such as *Mathematica*, one can define the functions as sums with the summation index varying from 0 to ∞ and the software will then automatically translate those sums into more standard hypergeometric notation as the functions ${}_pF_q$ defined below. But, be aware that many awkward things might happen as will be explained.

To get a grip on the situation let us begin by defining the *Pochhammer symbol*

$$(\alpha)_r := \frac{\Gamma(\alpha + r)}{\Gamma(\alpha)} = (\alpha)(\alpha+1)\cdots(\alpha+r-1) \tag{A.2}$$

for r a nonnegative integer. We have in particular, $(1)_n = n!$. The most common notation for a general Hypergeometric function with $p+q$ parameters is then the following:

$${}_pF_q\left(\begin{matrix} a_1 & \dots & a_p \\ b_1 & \dots & b_q \end{matrix}\middle| x\right) := \sum_{k=0}^{+\infty} \frac{(a_1)_k \cdots (a_p)_k}{(b_1)_k \cdots (b_q)_k k!} x^k. \tag{A.3}$$

Notice the extra $k!$ in the denominator. There are actually $q+1$ factorials in the denominator. This is the first awkward thing. If there is no $k!$ in the denominator we have to add it by hand by also adding another

$k!$ to the numerator and hence we must add a needless parameter just because of the bad notation.

The second problem is that if we have a simple term like $(k+n)!$, where n is a natural number, in the Taylor coefficient, then, since $(k+n)! = (n+1)_k \cdot n!$, we have to take $n!$ out of the sum and we get a $+1$ in the parameter. For example,

$$\sum_{k=0}^{+\infty} \frac{1}{k!(k+n)!} x^k = \frac{1}{n!} \sum_{k=0}^{+\infty} \frac{1}{k!(n+1)_k} x^k = \frac{1}{n!}\, {}_0F_1 \left(\begin{matrix} - \\ n+1 \end{matrix} \middle| x \right). \tag{A.4}$$

There are actually two problems here. The $1/n!$ factor and the awkward $+1$.

The last problem, for now, is that if we have a factorial of $2k$ instead of k, using the Pochhammer symbol, results in us having to divide in cases according to the parity of the parameter:

$$\begin{aligned} (2k+2n)! &= 2^{2k+n} n! n! (n+1)_k \left(n + \frac{1}{2}\right)_k \\ (2k+2n+1)! &= 2^{2k+n} n! (n+1)! (n+1)_k \left(n + \frac{3}{2}\right)_k . \end{aligned} \tag{A.5}$$

This is not just an awkward thing, but a real nuisance. To implement in *Mathematica* a function with a term like this, one must substitute n by a concrete number.

There are other possible notations for Hypergeometric functions. Let us examine them. The first alternative is the Meijer G-function. It has four sets of parameters, $G^{m,n}_{p,q}$, which for our purposes we will reduce to two:

$$G^{1,n}_{n,q} \left(\begin{matrix} a_1 & a_2 & \dots & a_n \\ 0 & b_2 & \dots & b_q \end{matrix} \middle| x \right) := \frac{1}{2\pi i} \int_L ds \frac{\Gamma(-s)\Gamma(1-a_1+s)\cdots\Gamma(1-a_n+s)}{\Gamma(1-b_2+s)\cdots\Gamma(1-b_q+s)} x^s \tag{A.6}$$

where L is an appropriate contour in the complex plane. What is important in this definition is the *sum over residues* in one side of the plane that is implicit, since the integral might not even converge. Supposing the parameters are all negative and recalling the fact that the poles of the Γ function are at the negative integers $-n$, including 0, and its residues are $(-1)^n n!$, we have:

$$G^{1,n}_{n,q} \left(\begin{matrix} a_1 & a_2 & \dots & a_n \\ 0 & b_2 & \dots & b_q \end{matrix} \middle| x \right) = \sum_{k=0}^{+\infty} \frac{(k-a_1)! \cdots (k-a_n)!}{k!(k-b_2)! \cdots (k-b_q)!} (-x)^k. \tag{A.7}$$

We have gotten rid of the $+1$ problem and the awkward normalization at the cost of now having a "$-$" sign in all the parameters. Since we will have factorials of $2k$ in some of our solutions the Meijer G-function is also not appropriate for our purposes. This leads us to the Fox H-function. Like the Meijer G-function it has four sets of parameters, $H^{m,n}_{p,q}$ that we will once again reduce to two:

$$H^{1,n}_{n,q} \left(\begin{matrix} (a_1,\alpha_1) & (a_2,\alpha_2) & \dots & (a_n,\alpha_n) \\ (0,1) & (b_2,\beta_2) & \dots & (b_q,\beta_q) \end{matrix} \middle| x \right) := \frac{1}{2\pi i} \int_L ds \frac{\Gamma(-s)\Gamma(1-a_1+\alpha_1 s)\cdots\Gamma(1-a_n+\alpha_n s)}{\Gamma(1-b_2+\beta_2 s)\cdots\Gamma(1-b_q+\beta_q s)} x^s, \tag{A.8}$$

where again L is an appropriate contour in the complex plane. Supposing the a_j's and b_j's are all negative we have:

$$H^{1,n}_{n,q}\left(\begin{matrix}(a_1,\alpha_1) & (a_2,\alpha_2) & \dots & (a_n,\alpha_n)\\ (0,1) & (b_2,\beta_2) & \dots & (b_q,\beta_q)\end{matrix}\middle| x\right) = \sum_{k=0}^{+\infty} \frac{(\alpha_1 k - a_1)!\cdots(\alpha_n k - a_n)!}{k!(\beta_2 k - b_2)!\cdots(\beta_q k - b_q)!}(-x)^k. \tag{A.9}$$

This is close to what we would want, but, again, we have the problem of the "$-$" sign in all the left parameters. Additionally, this function does not seem to be implemented in software packages.

A notation we shall use only in the simplest cases, is the Fox-Wright Ψ-function:

$${}_p\Psi_q\left(\begin{matrix}(a_1,\alpha_1) & \dots & (a_p,\alpha_p)\\ (b_1,\beta_2) & \dots & (b_q,\beta_q)\end{matrix}\middle| x\right) := \sum_{k=0}^{+\infty} \frac{\Gamma(\alpha_1 k + a_1)\cdots\Gamma(\alpha_p k + a_p)}{\Gamma(\beta_1 k + b_1)\cdots\Gamma(\beta_q k + b_q)k!}x^k. \tag{A.10}$$

Notice that once again we have an extra factorial $k!$ in the denominator as in the ${}_pF_q$. Also, since we are using the Γ function instead of factorials we will likewise have the problem of the $+1$ term in all the parameters. As with the Fox H-function, the Fox-Wright function does not seem to be implemented in software packages.

Having thus disposed of the question of the main notation, we will now discuss another problem with all the standard notations. For that we will introduce a **convention**: if n is a natural number then

$$\frac{1}{(-n)!} = 0. \tag{A.11}$$

This makes sense, since $\Gamma(-n+1) = \infty$, for n a natural number. This convention gives us an enormous freedom. For example, we can write an indefinite sum as a definite sum

$$\sum_{k=0}^{n} \frac{1}{k!(n-k)!} = \sum_{k=-\infty}^{+\infty} \frac{1}{k!(n-k)!}. \tag{A.12}$$

As definite integrals are easier to explicitly compute than indefinite ones, the same is true of definite and indefinite sums [27]. All of our solutions will be first given in the form of sums from $-\infty$ to $+\infty$ and only then will we present a sum starting at $k = 0$. This has the unfortunate problem of introducing cases. For example,

$$\sum_{k=-\infty}^{+\infty} \frac{1}{(k-a)!(k-b)!} \tag{A.13}$$

has two possible forms

$$\sum_{k=-\infty}^{+\infty} \frac{1}{(k-a)!(k-b)!} = \begin{cases} \sum_{k=0}^{+\infty} \frac{1}{k!(k+a-b)!} & \text{if } a \geq b \\ \sum_{k=0}^{+\infty} \frac{1}{k!(k+b-a)!} & \text{if } b \geq a. \end{cases} \tag{A.14}$$

Since we are interested in producing a bridge to the standard notation we will, as stated above, present power series as sums from 0 to ∞, but, from the typesetting point of view trying to write a definition by cases using power series or the standard notations is a nightmare. We will thus present the cases in the main text and not on the formulas.

A.1 Mellin Transform

Both the Meijer G-function and the Fox H-function have the form of inverse Mellin transforms. The *Mellin transform* of a function $f(x)$ is defined by

$$\tilde{f}(z) = \text{MT}[f(x); z] = \int_0^\infty dx f(x) x^{z-1}. \tag{A.15}$$

Together with an expression for $\tilde{f}(z)$, a vertical strip where the Mellin transform is analytic must be specified, the "*strip of analyticity*" (SOA). For example, if $f(x) = e^{-x}$ then $\tilde{f}(z) = \Gamma(z)$ and the SOA is given by the condition Re$(z) > 0$. The *inverse Mellin transform* is defined by

$$f(x) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} dz \tilde{f}(z) x^{-z}, \tag{A.16}$$

where the integration path is a vertical line lying within the SOA. If $\tilde{f}(z) = \Gamma(z)$ and the SOA is given by Re$(z) > 0$ then $f(x) = e^{-x}$, as expected. But, if instead the SOA was given by the condition $-1 <$ Re$(z) < 0$, then $f(x) = e^{-x} - 1$. If the integration path is more to the left we will have less poles over whose residues we will sum over.

The idea of the inverse Mellin transform is more general than the Mellin transform. For example, if $f(x) = e^x$ this function has no Mellin transform, but if we think on $\tilde{f}(z) = \Gamma(z)\cos(\pi z)$, then summing over the residues we get the right result. That is,

$$f(x) = \frac{1}{2\pi i} \int_L dz \Gamma(z) \cos(\pi z) x^{-z}, \tag{A.17}$$

but now L is not a vertical contour, it must have an inclination in the upper and lower left quadrants to accommodate the fact that $\cos(z)$ grows exponentially in the vertical direction. This type of analysis is very tedious and we will never engage in it. The main properties of the Mellin transform that will interest us are

$$\text{MT}[x^\alpha f(x); z] = \tilde{f}(z + \alpha) \tag{A.18}$$

$$\text{MT}[f(\alpha x); z] = \alpha^{-z} \tilde{f}(z) \tag{A.19}$$

$$\text{MT}[f(x^\alpha); z] = \frac{1}{|\alpha|} \tilde{f}\left(\frac{z}{\alpha}\right), \tag{A.20}$$

where the SOAs are accordingly transformed. Thinking in terms of power series of functions and of the inverse Mellin transform in terms of sums over residues these properties are all natural. For completeness we also give the Mellin transform of the product of two functions

$$\text{MT}[f(x)g(x); z] = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} dw \tilde{f}(w) \tilde{g}(z - w), \tag{A.21}$$

where a belongs to the SOA of $\tilde{f}(w)$. The integral on the right is an example of a *Mellin convolution*.

A.2 Bessel function cheat sheet

In this section we gather the facts about Bessel functions that will be used in the main text (see [26, 28, 29]). We start with the power series that defines a Bessel function

$$J_n(z) = \left(\frac{z}{2}\right)^n \sum_{k=0}^{\infty} \frac{(-1)^k z^{2k}}{4^k k!(k+n)!}. \tag{A.22}$$

Bessel functions of even index are even and Bessel functions of odd index are odd. This can be summarized as $J_n(-z) = (-1)^n J_n(z)$. As a result of our conventions we have that $J_{-n}(z) = (-1)^n J_n(z)$. Bessel functions satisfy the following identities

$$2nJ_n(z) = zJ_{n-1}(z) + zJ_{n+1}(z), \tag{A.23}$$

$$2J_n'(z) = J_{n-1}(z) - J_{n+1}(z). \tag{A.24}$$

Many Bessel function identities are proved from the generating function

$$e^{\frac{x}{2}\left(z-\frac{1}{z}\right)} = \sum_{n=-\infty}^{\infty} J_n(x) z^n, \tag{A.25}$$

of which, making $z = e^{i\theta}$, the Fourier series

$$e^{ix\sin(\theta)} = \sum_{n=-\infty}^{\infty} J_n(x) e^{in\theta} \tag{A.26}$$

is a particular case. From the unitarity of the Fourier transform we get

$$\sum_{n=-\infty}^{\infty} J_n(z)^2 = 1. \tag{A.27}$$

The product of Bessel functions is also a hypergeometric function

$$J_n(z)J_m(z) = \left(\frac{z}{2}\right)^{n+m} \sum_{k=0}^{\infty} \frac{(-1)^k (2k+n+m)! z^{2k}}{4^k k!(k+n)!(k+m)!(k+n+m)!}. \tag{A.28}$$

Finally, a particular case of Graf's formula will be implicitly present

$$J_n(2z\cos(\theta)) = \sum_{\substack{l \text{ same} \\ \text{parity as } n}} J_{\frac{n+l}{2}}(z) J_{\frac{n-l}{2}}(z) e^{il\theta}. \tag{A.29}$$

Appendix B

Coordinate transformations

In section 3.5 we will compute the Wigner transforms of solutions of the Helmholtz eq. in modified elliptic coordinates. In order to do that a few remarks are required. Using (2.43) and (2.97) we see that the Wigner transform of any integral kernel is given by

$$a(\theta, m) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta' e^{-im\theta'} K(\theta+\theta', \theta-\theta'), \tag{B.1}$$

so we have to be able to compute $K(\theta+\theta', \theta-\theta')$.

Starting from the solutions in polar coordinates $K(\theta_1, \theta_2) = u(r, \phi) = J_{2p}(\Omega r)\cos(2p\phi)$, and $K(\theta_1, \theta_2) = u(r, \phi) = J_{2p}(\Omega r)\sin(2p\phi)$ one has to first work out r, $\cos(2p\phi)$ and $\sin(2p\phi)$ in terms of θ_1 and θ_2. Starting with r:

$$\begin{aligned} r =& \sqrt{x^2+y^2} = \sqrt{\cos^2(\theta_1/2)\cos^2(\theta_2/2) - \sin^2(\theta_1/2)\sin^2(\theta_2/2)} \\ =& \frac{1}{\sqrt{2}}\sqrt{\cos(\theta_1)+\cos(\theta_2)}. \end{aligned} \tag{B.2}$$

Now, for the angular variables, we have by definition, that the Chebyshev polynomials of the first kind $T_n(x)$ and second kind $U_n(x)$ satisfy

$$T_n(\cos(\phi)) = \cos(n\phi) \quad \text{and} \quad U_n(\cos(\phi))\sin(\phi) = \sin((n+1)\phi), \tag{B.3}$$

respectively. Moreover,

$$\cos(\phi) = \frac{x}{r} = \frac{\sqrt{2}\cos(\theta_1/2)\cos(\theta_2/2)}{\sqrt{\cos(\theta_1)+\cos(\theta_2)}} \quad \text{and} \quad \sin(\phi) = \frac{y}{r} = \frac{i\sqrt{2}\sin(\theta_1/2)\sin(\theta_2/2)}{\sqrt{\cos(\theta_1)+\cos(\theta_2)}}, \tag{B.4}$$

hence

$$\cos(2p\phi) = T_{2p}\left(\frac{\sqrt{2}\cos(\theta_1/2)\cos(\theta_2/2)}{\sqrt{\cos(\theta_1)+\cos(\theta_2)}}\right) \tag{B.5}$$

and

$$\sin(2p\phi) = U_{2p-1}\left(\frac{\sqrt{2}\cos(\theta_1/2)\cos(\theta_2/2)}{\sqrt{\cos(\theta_1)+\cos(\theta_2)}}\right)\frac{i\sqrt{2}\sin(\theta_1/2)\sin(\theta_2/2)}{\sqrt{\cos(\theta_1)+\cos(\theta_2)}}. \tag{B.6}$$

The following trigonometric identities will be used

$$\cos(\theta+\theta') + \cos(\theta-\theta') = 2\cos(\theta)\cos(\theta') \tag{B.7}$$

$$\cos\left(\frac{\theta+\theta'}{2}\right)\cos\left(\frac{\theta-\theta'}{2}\right) = \frac{1}{2}\left(\cos(\theta)+\cos(\theta')\right) \tag{B.8}$$

$$\sin\left(\frac{\theta+\theta'}{2}\right)\sin\left(\frac{\theta-\theta'}{2}\right) = \frac{1}{2}\left(\cos(\theta')-\cos(\theta)\right) \tag{B.9}$$

We will also have a need of the following identities regarding Chebyshev polynomials:

$$T_n\left(\frac{x+y}{2\sqrt{xy}}\right) = \frac{1}{2}\left(\frac{x^{n/2}}{y^{n/2}} + \frac{y^{n/2}}{x^{n/2}}\right), \tag{B.10}$$

and

$$U_{2n+1}\left(\frac{x+y}{2\sqrt{xy}}\right) = \sum_{j=0}^{n}\frac{x^{j+1/2}}{y^{j+1/2}} + \sum_{j=0}^{n}\frac{y^{j+1/2}}{x^{j+1/2}}. \tag{B.11}$$

These identities are possibly new, but can be straightforwardly demonstrated from the recursion relations for Chebishev polynomials

$$T_{n+2}(x) = 2xT_{n+1}(x) - T_n(x) \quad \text{and} \quad U_{n+2}(x) = 2xU_{n+1}(x) - U_n(x) \tag{B.12}$$

with $T_0(x) = 1$, $T_1(x) = x$, $U_0(x) = 1$ and $U_1(x) = 2x$, plus the auxiliary formula

$$U_{2n}\left(\frac{x+y}{2\sqrt{xy}}\right) = \sum_{j=0}^{n}\frac{x^j}{y^j} + \sum_{j=0}^{n}\frac{y^j}{x^j} - 1, \tag{B.13}$$

which is also proved by recursion.

We are now ready to compute $K(\theta+\theta', \theta-\theta')$. Beginning with the simplest case $p = 0$,

$$K(\theta_1, \theta_2) = J_0[(\Omega/\sqrt{2})\sqrt{\cos(\theta_1)+\cos(\theta_2)}], \tag{B.14}$$

we only have to use (B.7) to get the expression that will be used in section 3.5

$$K(\theta+\theta', \theta-\theta') = J_0[\Omega\sqrt{\cos(\theta)\cos(\theta')}]. \tag{B.15}$$

Moving on to the general case $p \geq 0$, in the case of cosines we have

$$K(\theta_1, \theta_2) = J_{2p}[(\Omega/\sqrt{2})\sqrt{\cos(\theta_1)+\cos(\theta_2)}]\ T_{2p}\left(\frac{\sqrt{2}\cos(\theta_1/2)\cos(\theta_2/2)}{\sqrt{\cos(\theta_1)+\cos(\theta_2)}}\right), \tag{B.16}$$

and one obtains, using (B.7), (B.8) and (B.10),

$$K(\theta+\theta', \theta-\theta') = \frac{1}{2}J_{2p}[\Omega\sqrt{\cos(\theta)\cos(\theta')}]\left[\frac{\cos^p(\theta)}{\cos^p(\theta')} + \frac{\cos^p(\theta')}{\cos^p(\theta)}\right]. \tag{B.17}$$

In the case of sines, we have

$$K(\theta_1,\theta_2) = J_{2p}[(\Omega/\sqrt{2})\sqrt{\cos(\theta_1)+\cos(\theta_2)}]\; U_{2p-1}\left(\frac{\sqrt{2}\cos(\theta_1/2)\cos(\theta_2/2)}{\sqrt{\cos(\theta_1)+\cos(\theta_2)}}\right)\frac{i\sqrt{2}\sin(\theta_1/2)\sin(\theta_2/2)}{\sqrt{\cos(\theta_1)+\cos(\theta_2)}}, \tag{B.18}$$

and with some surprising cancelling of terms, using (B.7), (B.8), (B.9) and (B.11), we get

$$K(\theta+\theta',\theta-\theta') = \frac{i}{2}J_{2p}[\Omega\sqrt{\cos(\theta)\cos(\theta')}]\left[\frac{\cos^p(\theta')}{\cos^p(\theta)} - \frac{\cos^p(\theta)}{\cos^p(\theta')}\right]. \tag{B.19}$$