Applications of the Wigner function to quantum problems involving angle variables

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Abstract

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

1. Introduction

In the early years of quantum mechanics it was already observed by Condon [1] that the time-independent Schrödinger equation with the pendulum's potential corresponded to the Mathieu equation of classical mathematical physics [2, 3, 4], the eigenfunctions of the quantum pendulum (QP) being the Mathieu functions of even order. In the thesis this problem is studied in the Wigner-function representation and in the Density Operator representation. Perhaps surprisingly, closed forms for several families of stationary observables are presented.

The function carrying his name was initially defined by Wigner [5] for position/momentum variables and was subsequently modified by Berry [6] to accommodate angle/angular-momentum variables, a nontrivial problem even in the Schrödinger–Heisenberg setting, as reviewed by Carruthers and Nieto [7]. Later, Bizarro [8] found a modification of Berry's Wigner function that allowed the computation of the Moyal bracket [9, 10, 11]. Unfortunately, the general expressions derived by Bizarro [8] are too intricate, even more than in the position/momentum case, although the final equations for specific Hamiltonians turn out to be much simpler. It is shown, in Chapter 2, that the reason behind this contrasting behaviour is the simple form of the modified Wigner function when written in terms of Fourier coefficients.

In Chapter 3, closed forms for several families of stationary Wigner functions are presented that correspond to Hermitian operators (hence to observables), the closed expressions for the Fourier coefficients of the Wigner functions being then transformed into closed forms for the matrix elements of the corresponding observables in Chapter 4. Substituting the absolute value of the angular momentum by a (nonphysical) linear dependence on the latter in the Hamiltonian of a hindered rotator (HR) introduced by Berry [6] and extensively studied by Bizarro [8], an integrable model is obtained that shall be called the simplified HR (SHR). The SHR is such that the approximate formulas derived by Bizarro [8] for the HR become exact for the SHR, so the latter serves as a basis to study the QP since, to go from one model to the other, one just transforms a linear dependence on the angular momentum into a quadratic dependence. Moreover, the computations involved in the SHR are entirely analogous to the ones in the QP, but simpler, so, in Chapters 3 and 4, computations for the SHR model are always presented before those for the QP.

In the last 150 years [12], no closed forms were obtained for the Mathieu functions, even though they are as natural to appear, when dealing with elliptic coordinate problems [2, 3, 4, 13], as are Bessel functions in cylindrical coordinates [13, 14, 15, 16]. Now, the problem of finding closed forms for the Mathieu functions of even order, that is, closed forms for the Fourier coefficients of these functions (the so-called Mathieu coefficients), is actually equivalent to the problem of finding closed forms for the matrix elements of pure states, and in Chapter 4 several ideas to try to tackle this problem are analized. Finally, Chapter 5 ends with a summary and conclusions. The sections in this Extended Abstract follow roughly the chapters in the thesis.

2. Background

2.1. Brief review of the Wigner transform

From the wave function $|\psi\rangle$, Wigner [5] defined a function $W(x,p)$ in phase space that has the property that the marginal probabilities are the quantum probabilities:

$$\int_{-\infty}^{+\infty} dp\ W(x,p) = |\langle x|\psi\rangle|^2 = |\psi(x)|^2 \tag{1}$$

and

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

There are an infinite number of functions with this property, yet the one defined by Wigner, namely,

$$\begin{aligned} W(x,p) &= \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dx' e^{\frac{i}{\hbar}px'}\langle x-\tfrac{x'}{2}|\psi\rangle\langle\psi|x+\tfrac{x'}{2}\rangle \\ &= \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dp' e^{\frac{i}{\hbar}p'x}\langle p+\tfrac{p'}{2}|\psi\rangle\langle\psi|p-\tfrac{p'}{2}\rangle. \end{aligned} \tag{3}$$

has a certain number of extra properties that make it unique [17, 18].

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 have only allowed values $l = m\hbar$, 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 [6] defined the Wigner function

$$W(\theta,m) = \frac{1}{2\pi}\int_{-\pi}^{+\pi} d\theta' e^{im\theta'}\langle\theta-\tfrac{\theta'}{2}|\psi\rangle\langle\psi|\theta+\tfrac{\theta'}{2}\rangle, \tag{4}$$

which can also be found in Mukunda [19] and in Berman and Kolovsky [20]. With this expression one obtains the right marginals:

$$\sum_{m=-\infty}^{+\infty} W(\theta,m) = |\langle\theta|\psi\rangle|^2 \tag{5}$$

and

$$\int_{-\pi}^{+\pi} d\theta\ W(\theta,m) = |\langle m|\psi\rangle|^2. \tag{6}$$

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 $\hat{\rho} = |\psi\rangle\langle\psi|$:

$$A(\theta,m) = \frac{1}{2\pi}\int_{-\pi}^{+\pi} d\theta' e^{im\theta'}\langle\theta-\tfrac{\theta'}{2}|\hat{A}|\theta+\tfrac{\theta'}{2}\rangle. \tag{7}$$

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 final expression for the Moyal bracket in the standard position/momentum case turning out to be actually simpler than the expression for the Moyal product, due to cancelling of terms [9, 10].

In the case of angle/angular-momentum variables no such formula is known, which led Bizarro [8] 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:

$$w(\theta,m) = \frac{1}{2\pi}\sum_{\substack{m' \text{ same} \\ \text{parity as } m}} e^{i\theta m'}\langle\tfrac{m+m'}{2}|\psi\rangle\langle\psi|\tfrac{m-m'}{2}\rangle. \tag{8}$$

This transform was first defined by Chan [21] in the context of signal processing, when looking for alias-free time-frequency representations of discrete-time signals [22]. Here we find preferable to work with even and odd integers, rather than with integer and semi-integers [8], 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:

$$\sum_{m=-\infty}^{+\infty} w(\theta,m) = |\langle\theta|\psi\rangle|^2 \tag{9}$$

and

$$\int_{-\pi}^{+\pi} d\theta\ w(\theta,m) = \begin{cases} |\langle\frac{m}{2}|\psi\rangle|^2 & \text{if } m \text{ even} \\ 0 & \text{if } m \text{ odd} \end{cases} \tag{10}$$

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

$$w(\theta,2m) = \frac{W(\theta,m)+W(\theta+\pi,m)}{2}. \tag{11}$$

The modified Wigner transform (8) is immediately generalized to operators:

$$a(\theta,m) = \frac{1}{2\pi}\sum_{\substack{m' \text{ same} \\ \text{parity as } m}} e^{i\theta m'}\langle\tfrac{m+m'}{2}|\hat{A}|\tfrac{m-m'}{2}\rangle \tag{12}$$

and, while trying to obtain the evolution equation for the Wigner function, it was this modified Wigner transform that was used by Bizarro [8] to implicitly achieve formulas for the Moyal bracket. 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 [8] and compare with Eqs. (4.36) and (4.37) therein), the explanation for this residing in the simple form of the modified Wigner transform in the angular momentum basis. This is why we always work with the angular-momentum basis from now on, 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 $\hat{l} = -i\hbar\partial/\partial\theta$.

For future reference we give the formula for the integral form of the Moyal product of modified Wigner transforms

$$a\bigstar b(\theta,m) = \frac{1}{2\pi}\int_0^{2\pi} d\theta' \int_0^{2\pi} d\theta'' \sum_{\substack{m',m'':\\ m'+m''\text{ same}\\ \text{parity as } m}} a(\theta+\theta', m+m')b(\theta+\theta'', m+m'') \times e^{i(\theta' m''-\theta'' m')}. \tag{13}$$

This formula is new.

2.2. The Evolution Equations

The two models that will be studied are the *Simplified Hindered Rotator* (SHR)

$$\hat{H} = \omega\hat{l} - \lambda\cos(\hat{\theta}) \tag{14}$$

and the *Quantum Pendulum* (QP)

$$\hat{H} = \frac{\hat{l}}{2I} - \lambda\cos(\hat{\theta}). \tag{15}$$

From the equation giving the evolution of the density operator

$$i\hbar\frac{d}{dt}\hat{\rho}(t) = [\hat{H}, \hat{\rho}(t)], \tag{16}$$

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

$$i\hbar\frac{d\hat{\rho}_{r,s}}{dt} = [\hat{H},\hat{\rho}]_{r,s}, \tag{17}$$

one obtains the equations for the evolution of the matrix elements. These are

$$i\hbar\frac{d\hat{\rho}_{r,s}}{dt} = \hbar\omega(r-s)\hat{\rho}_{r,s} - \frac{\lambda}{2}(\hat{\rho}_{r-1,s} + \hat{\rho}_{r+1,s} - \hat{\rho}_{r,s+1} - \hat{\rho}_{r,s-1}) \tag{18}$$

for the SHR model and

$$i\hbar\frac{d\hat{\rho}_{r,s}}{dt} = \frac{\hbar^2}{2I}(r^2-s^2)\hat{\rho}_{r,s} - \frac{\lambda}{2}(\hat{\rho}_{r-1,s} + \hat{\rho}_{r+1,s} - \hat{\rho}_{r,s+1} - \hat{\rho}_{r,s-1}) \tag{19}$$

for the QP model, respectively. Expanding the modified Wigner transform into a Fourier series

$$w(\theta,m,t) = \frac{1}{2\pi}\sum_{\substack{n\text{ same}\\ \text{parity as } m}} a_{m,n}(t)e^{in\theta}, \tag{20}$$

it is evident from (8) that the Fourier coefficients $a_{m,n}$ for m and n of the same parity are given by

$$a_{m,n}(t) = \langle \tfrac{m+n}{2}|\hat{\rho}(t)|\tfrac{m-n}{2}\rangle. \tag{21}$$

This allows an easier derivation of the evolution equation for the modified Wigner transforms. These read

$$\hbar\frac{\partial w}{\partial t}(\theta,m,t) = -\hbar\omega\frac{\partial w}{\partial\theta}(\theta,m,t) - \lambda\sin(\theta) \times [w(\theta,m-1,t) - w(\theta,m+1,t)] \tag{22}$$

in the case of the SHR model and

$$\hbar\frac{\partial w}{\partial t}(\theta,m,t) = -\frac{\hbar^2}{2I}m\frac{\partial w}{\partial\theta}(\theta,m,t) - \lambda\sin(\theta) \times [w(\theta,m-1,t) - w(\theta,m+1,t)] \tag{23}$$

in the QP case. These equations can also be obtained from the integral form for the Moyal product (13) in a manner that is much easier than the use of the differential form of the Moyal bracket as was done in [8].

2.3. Mathieu functions and the Helmholtz equation

The eigenfunctions of the SHR model have the form of Frequency-Modulated signals

$$\psi(\theta) = \frac{1}{\sqrt{2\pi}}e^{i\frac{E}{\hbar\omega}\theta}e^{i\frac{\lambda}{\hbar\omega}\sin(\theta)} \tag{24}$$

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.

In the QP case, the eigenfunctions satisfy the equation

$$-\frac{\hbar^2}{2I}\frac{d^2\psi}{d\theta^2}(\theta) - \lambda\cos(\theta)\psi(\theta) = E\psi(\theta), \tag{25}$$

which is a particular case of the Mathieu equation whose standard form reads [1, 2, 3, 4, 23, 24]:

$$\frac{d^2f}{dz^2}(z) + [a - 2q\cos(2z)]f(z) = 0. \tag{26}$$

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 then becomes

$$4\frac{d^2\psi}{d\theta^2}(\theta) + [a - 2q\cos(\theta)]\psi(\theta) = 0 \tag{27}$$

and, comparing with (25), we see that $E = \hbar^2 a/8I$ and $q = -4\lambda I/\hbar^2$, the QP problem having been thus reduced to the study of the Mathieu functions of even order. Unfortunately, for 150 years of research no closed forms have yet been reached for the Mathieu functions of even order, so in what follows we discuss how to tackle this problem.

The Mathieu equation first appeared in the context of the Helmholtz equation in 2 dimensions

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \Omega^2 u = 0. \tag{28}$$

When one looks for stationary solutions to the evolution equation for the QP model (19) it will be found that the integral kernel of a stationary operator satisfies

$$\frac{\partial^2 K}{\partial \theta_1^2} - \frac{\partial^2 K}{\partial \theta_2^2} + \frac{2\lambda I}{\hbar^2}[\cos(\theta_1) - \cos(\theta_2)]K = 0. \tag{29}$$

Comparing this eq. with Helmholtz' equation in modified elliptic coordinates

$$\frac{\partial^2 u}{\partial z_1^2} - \frac{\partial^2 u}{\partial z_2^2} - \frac{\Omega^2}{2}[\cos(2z_1) - \cos(2z_2)]u = 0 \tag{30}$$

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

One then has that solutions of the Helmholtz equation in a given coordinate system when translated into modified elliptic coordinates (that is, substitute x by $\cos(\theta_1/2)\cos(\theta_2/2)$, y by $i\sin(\theta_1/2)\sin(\theta_2/2)$ and see if the result has period 2π in θ_1 and θ_2) give stationary solutions to the evolution equation for the QP model. The solutions that will be analized are: the simplest solution in cartesian coordinates $K(\theta_1,\theta_2) = \cos(\Omega x)$; and the family of solutions in polar coordinates

$$K(\theta_1,\theta_2) = J_{2p}(\Omega r)e^{\pm i2p\phi}, \tag{31}$$

where p is a natural number.

3. Stationary solutions - Wigner function

Making the right-hand side of (22) equal to 0, after replacing $w(\theta,m)$ with $a(\theta,m)$, we have

$$\frac{\partial a}{\partial \theta}(\theta,m) = -\frac{\lambda}{\hbar\omega}\sin(\theta)[a(\theta,m-1) - a(\theta,m+1)], \tag{32}$$

and so, defining as in Bizarro [8] $y = 2(\lambda/\hbar\omega)\cos(\theta)$ and $Z(y,m) = a(\theta,m)$, we get

$$2\frac{\partial Z}{\partial y}(y,m) = Z(y,m-1) - Z(y,m+1) \tag{33}$$

for the SHR. In the case of the QP, the right-hand side of (23) gives

$$m\frac{\partial a}{\partial \theta}(\theta,m) = -2\frac{\lambda I}{\hbar^2}\sin(\theta)[a(\theta,m-1) - a(\theta,m+1)], \tag{34}$$

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

$$m\frac{\partial Z}{\partial y}(y,m) = Z(y,m+1) - Z(y,m-1). \tag{35}$$

3.1. Simplest solutions - continuous family

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

$$Z(y,m) = e^y f(m), \tag{36}$$

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 $Z(y,m)$:

$$Z(y,m) = e^{\alpha y} f(m). \tag{37}$$

The equations for the SHR and QP models become respectively:

$$\alpha 2 f(m) = f(m-1) - f(m+1) \tag{38}$$

and

$$\alpha m f(m) = f(m+1) - f(m-1). \tag{39}$$

In the first case we have a second order difference equation with constant coefficients. In the second case we must solve a second order difference equation with variable coefficents. There are standard methods for solving them [25]. We get in the first case

$$f(m) = (-\alpha \pm \sqrt{\alpha^2+1})^m, \tag{40}$$

and in the second case

$$f(m) = i^m J_m\left(\frac{2i}{\alpha}\right). \tag{41}$$

The corresponding families of Wigner functions are given by linear combinations of solutions. Not all these solutions are Wigner transforms of operators. From the definition (12) 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

$$\begin{aligned} a_\alpha(\theta, m) =& e^{2\alpha(\lambda/\hbar\omega)\cos(\theta)}(-\alpha \pm \sqrt{\alpha^2+1})^m \\ &+ e^{-2\alpha(\lambda/\hbar\omega)\cos(\theta)}(+\alpha \mp \sqrt{\alpha^2+1})^m, \end{aligned} \tag{42}$$

and for the Quantum Pendulum by

$$\begin{aligned} a_\alpha(\theta, m) =& e^{-2\alpha(\lambda I/\hbar^2)\cos(\theta)} i^m J_m\left(\frac{2i}{\alpha}\right) \\ &+ e^{2\alpha(\lambda I/\hbar^2)\cos(\theta)} i^m J_m\left(\frac{2i}{-\alpha}\right). \end{aligned} \tag{43}$$

3.2. Two discrete variables

In solving (33), and despite the fact that Bizarro [8] 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:

$$Z(y, m) = \sum_{j=-\infty}^{\infty} X(m, j) y^j \tag{44}$$

and, equating terms in (33), we get an equation for $X(m, j)$:

$$2(j+1)X(m, j+1) = X(m-1, j) - X(m+1, j). \tag{45}$$

Coming now to the main trick to solve this type of equation, which is separation of variables [25], we assume that

$$X(m, j) = f(j-m)g(j+m) \tag{46}$$

and get

$$\begin{aligned} 2(j+1)&f(j+1-m)g(j+1+m) \\ &= f(j-m+1)g(j+m-1) \\ &\quad - f(j-m-1)g(j+m+1). \end{aligned} \tag{47}$$

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

$$\begin{aligned} (n+k+2)f(n+1)g(k+1) =& f(n+1)g(k-1) \\ &- f(n-1)g(k+1) \end{aligned} \tag{48}$$

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

$$n+1+\frac{f(n-1)}{f(n+1)} = -k-1+\frac{g(k-1)}{g(k+1)}. \tag{49}$$

For (49) 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

$$f(n+2) = \frac{-1}{(n+2)-D} f(n), \tag{50}$$

of which a solution is

$$f(n) = \frac{(-1)^{\frac{n}{2}}}{2^{\frac{n}{2}}\left(\frac{n}{2}-d\right)!}, \tag{51}$$

when n is even and $f(n) = 0$, otherwise. Similarly, from the right-hand side of (49) being equal to the same constant D, we get

$$g(k+2) = \frac{1}{k+2+D} g(k), \tag{52}$$

and the same reasoning gives us

$$g(k) = \frac{1}{2^{\frac{k}{2}}\left(\frac{k}{2}+d\right)!}, \tag{53}$$

for k even and $g(k) = 0$, otherwise. Substituting in (44), yields

$$Z(y, m) = \sum_{\substack{j \text{ same} \\ \text{parity as } m}} \frac{(-1)^{\frac{j-m}{2}}}{2^j\left(\frac{j-m}{2}-d\right)!\left(\frac{j+m}{2}+d\right)!} y^j, \tag{54}$$

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 (54) 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,

$$Z(y, m) = J_{m+2d}(y) \tag{55}$$

is a solution to (33), something that is well known [14, 15, 16]. Finally, we have the following family of solutions to the stationarity equation for the SHR model:

$$a_{2d}(\theta, m) = J_{m+2d}\left(\frac{2\lambda}{\hbar\omega}\cos(\theta)\right). \tag{56}$$

Modulo a 2π factor and changing d to $-d$, this is the Wigner transform of (24).

This was for the SHR model, in the case of the QP model this time $X(m, j)$ must satisfy the equation

$$m(j+1)X(m, j+1) = X(m+1, j) - X(m-1, j). \tag{57}$$

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

$$X(m, j) = f(j-m)g(j+m)h(j) \tag{58}$$

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

$$Z(y,m) = (-1)^m y^{|m|+2d} \times \sum_{k=0}^{\infty} \frac{1}{k!(k+|m|)!(2k+|m|+2d)!} y^{2k}, \tag{59}$$

and the second

$$Z(y,m) = (-1)^m y^{|m|+|2d|} \sum_{k=0}^{\infty} \frac{1}{k!(k+|2d|)!} \times \frac{1}{(k+|m|)!(k+|m|+|2d|)!} y^{2k}. \tag{60}$$

3.3. Three discrete variables
Instead of trying to solve equations (32) and (34) as in the previous section, we work here directly with the Fourier coefficients of the Wigner transforms and equate the right-hand sides of (22) and (23) to 0. More precisely, we try to solve

$$\hbar\omega n a_{m,n} = \frac{\lambda}{2}(a_{m-1,n-1} + a_{m+1,n+1} - a_{m+1,n-1} - a_{m-1,n+1}) \tag{61}$$

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

$$n a_{m,n} = -c(a_{m-1,n-1} + a_{m+1,n+1} - a_{m+1,n-1} - a_{m-1,n+1}). \tag{62}$$

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

$$\frac{\hbar^2}{2I} mn a_{m,n} = \frac{\lambda}{2}(a_{m-1,n-1} + a_{m+1,n+1} - a_{m+1,n-1} - a_{m-1,n+1}), \tag{63}$$

or

$$mn a_{m,n} = -c(a_{m-1,n-1} + a_{m+1,n+1} - a_{m+1,n-1} - a_{m-1,n+1}), \tag{64}$$

if we define $c = -\lambda I/\hbar^2$. As in the previous section, we expand the Fourier coefficients in a power series, but use the constants c instead of y:

$$a_{m,n} = \sum_{j=0}^{\infty} Y(m,n,j) c^j, \tag{65}$$

so that, from (62), the equation for $Y(m,n,j)$ becomes

$$\begin{aligned} nY(m,n,j) = &- Y(m-1,n-1,j-1) \\ &- Y(m+1,n+1,j-1) \\ &+ Y(m+1,n-1,j-1) \\ &+ Y(m-1,n+1,j-1). \end{aligned} \tag{66}$$

For the QP, the only difference from (66) will be that we now have mn on the left-hand side instead of n. Again as in the previous section, we now attempt to do separation of variables and assume that

$$Y(m,n,j) = h(j+m)r(j-m)s(j+n)t(j-n)u(j). \tag{67}$$

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 (66) as

$$\begin{aligned} nh(k)r(l)s(p)t(q)u(j) &= -h(k-2)r(l)s(p-2)t(q)u(j-1) \\ &\quad - h(k)r(l-2)s(p)t(q-2)u(j-1) \\ &\quad + h(k)r(l-2)s(p-2)t(q)u(j-1) \\ &\quad + h(k-2)r(l)s(p)t(q-2)u(j-1). \end{aligned} \tag{68}$$

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

$$\begin{aligned} nu(j) = &- \left[\frac{h(k-2)s(p-2)}{h(k)s(p)} + \frac{r(l-2)t(q-2)}{r(l)t(q)} \right. \\ &\left. - \frac{r(l-2)s(p-2)}{r(l)s(p)} - \frac{h(k-2)t(q-2)}{h(k)t(q)}\right] \\ &\times u(j-1). \end{aligned} \tag{69}$$

In the QP case we get the same but for $mnu(j)$ on the left hand side. Making different hypothesis about $u(j)$ and substituting j by different combinations of k, l or p, q we get four families of solutions that depend on three parameters. In the QP case the first family is

$$Y^1_{j_0,d_1,d_2}(m,n,j) = \frac{(-1)^{j+j_0}}{\left(\frac{j+j_0+m+d_1}{2}\right)!\left(\frac{j+j_0-m+d_1}{2}\right)!} \times \frac{1}{\left(\frac{j+j_0+n+d_2}{2}\right)!\left(\frac{j+j_0-n+d_2}{2}\right)!}, \tag{70}$$

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

$$Y^2_{j_0,d_1,d_2}(m,n,j) = \frac{(-1)^{j+j_0}}{\left(\frac{j+j_0+m+d_1}{2}\right)!\left(\frac{j+j_0+m-d_1}{2}\right)!} \times \frac{(j+j_0)!}{\left(\frac{j+j_0-m+d_1}{2}\right)!\left(\frac{j+j_0-m-d_1}{2}\right)!} \times \frac{1}{\left(\frac{j+j_0+n+d_2}{2}\right)!\left(\frac{j+j_0-n+d_2}{2}\right)!}, \tag{71}$$

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

$$Y^3_{j_0,d_1,d_2}(m,n,j) = \frac{(-1)^{j+j_0}}{\left(\frac{j+j_0+m+d_1}{2}\right)!\left(\frac{j+j_0-m+d_1}{2}\right)!} \times \frac{(j+j_0)!}{\left(\frac{j+j_0+n+d_2}{2}\right)!\left(\frac{j+j_0+n-d_2}{2}\right)!} \times \frac{1}{\left(\frac{j+j_0-n+d_2}{2}\right)!\left(\frac{j+j_0-n-d_2}{2}\right)!}, \tag{72}$$

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

$$Y^4_{j_0,d_1,d_2}(m,n,j) = \frac{(-1)^{j+j_0}}{\left(\frac{j+j_0+m+d_1}{2}\right)!\left(\frac{j+j_0+m-d_1}{2}\right)!} \times \frac{(j+j_0)!}{\left(\frac{j+j_0-m+d_1}{2}\right)!\left(\frac{j+j_0-m-d_1}{2}\right)!} \times \frac{(j+j_0)!}{\left(\frac{j+j_0+n+d_2}{2}\right)!\left(\frac{j+j_0+n-d_2}{2}\right)!} \times \frac{1}{\left(\frac{j+j_0-n+d_2}{2}\right)!\left(\frac{j+j_0-n-d_2}{2}\right)!}, \tag{73}$$

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

3.4. Comparisons

To compare solutions obtained via the two approaches detailed in the previous two sections, we only have to calculate the Fourier coefficients for the solutions derived using the $y = 2\lambda/\hbar\omega\cos(\theta)$ and $y = -2\lambda I/\hbar^2\cos(\theta)$ variables 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. In the SHR case we get that the solutions in (56) are a subfamily of the third family of solutions with three discrete variables with parameters $j_0 = d_2 = 0$ and $d_1 = 2d$. In the QP case the family (59) corresponds to first family (70) with parameters $j_0 = d_2 = 0$ e $d_1 = -2d$. The family (60) corresponds to the second family (71) with parameters $j_0 = d_2 = 0$ and $d_1 = 2d$.

3.5. Wigner transforms of Helmholtz solutions

The Wigner transform of $K(\theta_1,\theta_2) = u(x,y) = \cos(\Omega x)$ gives

$$a(\theta,m) = \frac{1}{2}\left[i^m J_m\left(\frac{\Omega}{2}\right)e^{i\frac{\Omega}{2}\cos(\theta)} + i^m J_m\left(-\frac{\Omega}{2}\right)e^{-i\frac{\Omega}{2}\cos(\theta)}\right]. \tag{74}$$

Recalling that $\Omega^2 = -16\lambda I/\hbar^2$ we recognize in the expression inside square brackets the solution (43) with $\alpha = i4/\Omega$.

The Wigner transform of the simplest solution in polar coordinates $K(\theta_1,\theta_2) = u(r,\phi) = J_0(\Omega r)$ is

$$a(\theta,m) = \left(-\tfrac{\Omega^2}{8}\cos(\theta)\right)^{|m|}\sum_{k=0}^{\infty}\frac{(-\frac{\Omega^2}{8})^{2k}\cos^{2k}(\theta)}{k!(k+|m|)!} \times \frac{1}{(2k+|m|)!}. \tag{75}$$

This is (59) with $d = 0$. For the more general cases of $K(\theta_1,\theta_2) = u(r,\phi) = J_{2p}(\Omega r)\cos(2p\phi)$ and $K(\theta_1,\theta_2) = u(r,\phi) = J_{2p}(\Omega r)\sin(2p\phi)$ one can use identities involving Chebyshev polynomials to arrive at the result that the Wigner transforms of these Helmholtz solutions are linear combinations of the solutions in (59) with $d = p$ and $d = -p$. This will then imply that modulo a constant $K(\theta_1,\theta_2) = u(r,\phi) = J_{2p}(\Omega r)e^{i2p\phi}$ corresponds to (59) with $d = p$ and $K(\theta_1,\theta_2) = u(r,\phi) = J_{2p}(\Omega r)e^{-i2p\phi}$ to (59) with $d = -p$.

4. Stationary solutions - Density Operator

4.1. Matrix elements

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,

$$\langle r|\hat{A}|s\rangle = \sum_{j=-\infty}^{\infty} G(r,s,j)c^j, \tag{76}$$

and of equations (18) and (19) for the evolution of the density operator (with their left-hand sides set to zero), we obtain the following stationarity equations for $G(r,s,j)$:

$$\begin{aligned}(r-s)G(r,s,j) &= -G(r-1,s,j-1) - G(r+1,s,j-1)\\ &\quad + G(r,s+1,j-1) + G(r,s-1,j-1).\end{aligned} \tag{77}$$

and

$$\begin{aligned}(r^2-s^2)G(r,s,j) &= -G(r-1,s,j-1) - G(r+1,s,j-1)\\ &\quad + G(r,s+1,j-1) + G(r,s-1,j-1),\end{aligned} \tag{78}$$

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 (67) 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 translations in the parameter j_0 correspond to multiplying by an overall constant c^{-j_0} so we can forget about the dependence on j_0 and from (70), (71), (72), and (73), we have for the four families of 3.3 the corresponding families of stationary operators:

$$\langle r|\hat{A}^1_{d_1,d_2}|s\rangle = \sum_{\substack{j\text{ same}\\ \text{parity as}\\ r+s+d_1}} \frac{(-1)^j}{\left(\frac{j+r+s+d_1}{2}\right)!\left(\frac{j-r-s+d_1}{2}\right)!} \times \frac{1}{\left(\frac{j+r-s+d_2}{2}\right)!\left(\frac{j-r+s+d_2}{2}\right)!}c^j, \tag{79}$$

$$\langle r|\hat{A}^2_{d_1,d_2}|s\rangle = \sum_{\substack{j\text{ same}\\ \text{parity as}\\ r+s+d_1}} \frac{(-1)^j}{\left(\frac{j+r+s+d_1}{2}\right)!\left(\frac{j+r+s-d_1}{2}\right)!} \times \frac{j!}{\left(\frac{j-r-s+d_1}{2}\right)!\left(\frac{j-r-s-d_1}{2}\right)!} \times \frac{1}{\left(\frac{j+r-s+d_2}{2}\right)!\left(\frac{j-r+s+d_2}{2}\right)!}c^j, \tag{80}$$

$$\langle r|\hat{A}^3_{d_1,d_2}|s\rangle = \sum_{\substack{j\text{ same}\\ \text{parity as}\\ r+s+d_1}} \frac{(-1)^j}{\left(\frac{j+r+s+d_1}{2}\right)!\left(\frac{j-r-s+d_1}{2}\right)!} \times \frac{j!}{\left(\frac{j+r-s+d_2}{2}\right)!\left(\frac{j+r-s-d_2}{2}\right)!} \times \frac{1}{\left(\frac{j-r+s+d_2}{2}\right)!\left(\frac{j-r+s-d_2}{2}\right)!}c^j. \tag{81}$$

and

$$\langle r|\hat{A}^4_{j_0,d_1,d_2}|s\rangle = \sum_{\substack{j\text{ same}\\ \text{parity as}\\ r+s+d_1}} \frac{(-1)^j}{\left(\frac{j+r+s+d_1}{2}\right)!\left(\frac{j+r+s-d_1}{2}\right)!} \times \frac{j!}{\left(\frac{j-r-s+d_1}{2}\right)!\left(\frac{j-r-s-d_1}{2}\right)!} \times \frac{j!}{\left(\frac{j+r-s+d_2}{2}\right)!\left(\frac{j+r-s-d_2}{2}\right)!} \times \frac{1}{\left(\frac{j-r+s+d_2}{2}\right)!\left(\frac{j-r+s-d_2}{2}\right)!}c^j, \tag{82}$$

with $c = -\lambda I/\hbar^2$ and d_1 and d_2 always of the same parity in (79)–(82).

4.2. Pure states and Mathieu functions

Pure states are those states of the form $\hat{\rho} = |\psi\rangle\langle\psi|$. Stationary pure states are those pure states for which $|\psi\rangle$ is an eigenfunction of the Hamiltonian. In the case of the QP model these are the Mathieu functions $\psi(\theta) = ce_{2n}(\theta/2)$. 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,

$$\langle r|ce_{2n}\rangle\langle ce_{2n}|s\rangle = \sum_{j=-\infty}^{\infty} F^{(2n)}(r,s,j)c^j, \tag{83}$$

one would like to know if any of the solutions already found corresponds to any $F^{(2n)}$. To do that we must compare them with the Taylor coefficients, as functions of the coupling constant, of the Fourier coefficients of Mathieu functions. The Fourier coefficients of Mathieu functions are called Mathieu coefficients. The first non-zero Taylor coefficients of the Mathieu coefficients are known and they translate into the following boundary condition for $F^{(2n)}(r,s,j)$ when $r,s \geq n > 0$:

$$F^{(2n)}(r,s,r+s-2n) = \frac{1}{4}(-1)^{r+s-2n}\frac{(2n)!(2n)!}{(r-n)!(r+n)!(s-n)!(s+n)!}, \tag{84}$$

whereas

$$F^{(2n)}(r,s,j) = 0 \tag{85}$$

for $j < r+s-2n$. If $n=0$, we have the same expression, but without the factor 1/4. Looking at the solutions of the previous section and allowing translations in the parameter j_0 we find that we can verify the boundary conditions (84) and (85) with a member of the third family, $(2n)!^2 G^3_{2n,0,2n}/4$, 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 $G^3_{0,0,0}$. This is 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 $n>0$, 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 $n > r, s \geq 0$. 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, 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 satisifies the boundary conditions.

Since the solutions of the Helmholtz equation generate the space of functions generated by the products of 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

$$|ce_{2n}\rangle\langle ce_{2n}| = \sum_{d=-\infty}^{\infty} \alpha^n_d \hat{A}^1_{-d,2d,0}. \tag{86}$$

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

$$\alpha^n_d = \sum_k \alpha^n_{d,k} c^k, \tag{87}$$

we obtain the following decomposition

$$F^{(2n)} = \sum_{d=-\infty}^{\infty} \sum_k \alpha^n_{d,k}\, G^1_{-k-d,2d,0}. \tag{88}$$

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

$$\sum_{d,k} \alpha^0_{d,k}\, G^1_{-k-d,2d,0}(r, s, |r| + |s|) = \frac{(-1)^{r+s}}{|r|!|r|!|s|!|s|!}, \tag{89}$$

for all $r, s \in \mathbb{Z}$. An expression that works is

$$\alpha_{d,d} = \frac{1}{d!d!}. \tag{90}$$

and $\alpha_{d,k} = 0$ when $k < d$. The result of summing the right hand side of (88) with this expression for the coefficients $\alpha_{d,k}$ is

$$\sum_{d=-\infty}^{\infty} \alpha_{d,d} G^1_{-2d,2d,0} = G^3_{0,0,0} + G^2_{0,0,0} - G^1_{0,0,0}. \tag{91}$$

We had already seen that this linear combination satisfies the boundary conditions. To proceed further one must try to obtain a linear combination that satisfies the non-linear condition

$$\hat{\rho} \cdot \hat{\rho} = \hat{\rho} \tag{92}$$

an equation that is only satisfied by pure states.

5. Conclusions

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.

The most immediate work to be done in the future 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.

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