DEFORMATION QUANTIZATION FOR CONTACT INTERACTIONS AND DISSIPATION

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Contents

Abstract

This thesis studies deformation quantization and its application to contact interactions and systems with dissipation. We consider the subtleties related to quantization when contact interactions and boundaries are present. We exploit the idea that discontinuous potentials are idealizations that should be realized as limits of smooth potentials. The Wigner functions are found for the Morse potential and in the proper limit they reduce to the Wigner functions for the infinite wall, for the most general (Robin) boundary conditions. This is possible for a very limited subset of the values of the parameters — so-called fine tuning is necessary. It explains why Dirichlet boundary conditions are used predominantly. Secondly, we consider deformation quantization in relation to dissipative phenomena. For the damped harmonic oscillator we study a method using a modified noncommutative star product. Within this framework we resolve the non-reality problem with the Wigner function and correct the classical limit.

Chapter 1

Introduction

This thesis is a study of deformation quantization, also known as phase-space quantum mechanics. It is a method of quantization alternative to operator quantum mechanics and path integral quantization. In this framework phase space plays the central role, along with phase space probability distributions.[1] No operators or wave functions are needed. The physical observables are phase space functions, multiplied with a special non-commutative *star product* in order to take into account any non-commutative phenomena resulting from the quantum nature of the system of interest. The Wigner function is the deformation quantization counterpart of the wave function, since it corresponds to the state of the system and allows amplitudes and probabilities to be calculated. The equation of motion, i.e. the Moyal equation, can be solved to determine the Wigner function at any time. It involves the star product and it is a deformation of the classical equations with deformation parameter $\hbar$. More generally, the transition from classical to quantum mechanical description (algebra of observables, equations of motion, probability distributions) comes from generalizations of classical physics.

The original results of this paper are in two areas. We treat the infinite wall as the prototypical example of a contact interaction or system with a bounded domain.

[1] Strictly speaking *quasi-distributions*, since they have negative values.

The infinite wall is realized as a limit of smooth potentials, with all the possible boundary conditions emerging as different potentials are selected. Secondly we apply deformation quantization to dissipative systems, in this case to the damped harmonic oscillator, using a deformation of the star product to write the dynamical equation describing the evolution in terms of phase space quantum mechanics.

As an alternative approach, deformation quantization has been applied to already known systems, with the goal of recovering the known physics within the new framework. This involves solving the star-eigenvalue equations directly. What "directly" means is that we cannot exploit the relationships between the different quantization techniques. In some sense we want to pretend that we found deformation quantization first and that we have no idea that path integrals or operators and wave functions exist. Sometimes we refer to this program as "pure" deformation quantization.

However there is another important aspect that must be explored. In this thesis we test the ability of deformation quantization to provide successful and systematic treatment of extreme systems whose quantization is subtle regardless which method is used. This is why we study systems with bounded domains and systems with dissipation – they are extreme types of systems that will provide ideal testing ground for phase space quantum mechanics. The last was the primary motivation behind the results in this thesis. While phase space quantum mechanics has been established as an alternative quantization method without doubt, interesting results emerge when extreme systems are considered.

1.1 Contact interactions in operator and phase space quantum mechanics

Contact interactions are among the first quantum mechanical systems one encounters when studying quantum mechanics. Surprisingly they are highly nontrivial in phase

space. In operator quantum mechanics one can solve the Schrödinger equation piecewise for any potential that involves infinite walls, delta functions, finite potential steps and wells, etc. and then do matching by varying the constants of integration. For the Schrödinger equation this program is very effective. In deformation quantization, however one cannot hope to proceed in similar way due to a nontrivial interaction with the boundaries. The Wigner function for a bounded region does not satisfy the equations of motion for the Hamiltonian in the bulk and therefore the notion of matching is meaningless without modification.

In this thesis we concentrate on the simplest contact interaction – the infinite wall. Equivalently we can consider a particle confined to the half line. It is known that the boundary conditions imposed at zero can be one of the following: Dirichlet – when the wave function vanishes, Neumann – vanishing first derivative and Robin boundary conditions – a linear combinations of the previous two. The boundary conditions allowed can be derived if one insists on hermiticity of the Hamiltonian. More precisely a given Hamiltonian can be symmetric but not self adjoint. An unique self adjoint extension may exist or infinitely many extensions can be written depending on the operator. In the case of the infinite wall the Hamiltonian has infinitely many self-adjoint extensions each corresponding to a different linear combination of Dirichlet and Neumann boundary conditions. Different extensions lead to different physics, thus emphasizing the need of resolving this problem in deformation quantum mechanics.

The motivation for this work comes partly from the previous work [29]. The authors consider the infinite wall, i.e. a free particle confined on a half line. Their assumption is that the physical Wigner function can be obtained using the Wigner transform on the density matrix coming from the Schrödinger treatment. Using this as a starting point, they show that the Wigner function can be found from the star-eigenvalue equations if the Hamiltonian is modified to include boundary terms. This

way, similarly to the wave function counterpart, we can solve in the bulk and set the value of the Wigner function to zero at the origin. This program, however, is difficult to carry out in practical calculation for other potentials and is essentially a derivation from operator quantum mechanics. Also it is assumed that the Wigner transform does not change when systems of boundaries are involved, i.e. the symbol (under this transformation) of the density operator is the physical Wigner function. We need a justification from within the deformation quantization framework.

We argue that the infinite wall should be approached differently. Sharp potentials are understood as idealisations of physical, smooth potentials and so they should be realized as limits of such. Since deformation quantization reproduces the known result from operator quantum mechanics, as long as smooth potentials are involved, we can quantize any smooth potential without encountering the boundary problems. After the Wigner function is found we can take the limit to recover the infinite wall and observe the effect on the Wigner function. Can that program be carried out?

In [55] the Dirichlet boundary conditions are indeed recovered using Liouville potential. More generally, Šeba ([68]) produces Robin boundary conditions[2] for wave functions using a discontinuous potential. A natural choice then is the Morse potential. The Liouville potential is a particular case of the Morse potential, and its features resemble Šeba's potential. In addition it is exactly solvable. We find the Wigner function for the Morse potential and show that it recovers the Wigner function with Robin boundary conditions in a certain limit of the parameters. This provides a pure deformation quantization treatment of the infinite wall problem justifying the assumptions Dias and Prata made in [29].

The limit we study exhibits two interesting features – mass dependence and fine tuning. The first – mass dependence – means that the Morse potential's parameters

[2]Standard and non-standard walls are terms sometimes used for infinite walls for which the Dirichlet and Robin (excluding Dirichlet) boundary conditions are imposed on the wave functions at the origin.

need to be adjusted for different particles, i.e. they depend explicitly on the mass. By "fine tuning" we mean that for generic values of the potential parameters we recover Dirichlet boundary conditions. Only for very restricted values we realize non-standard walls. These two interesting phenomena also occur in the Šeba case. Also if one uses a finite discontinuous potential as in [38], mass dependence and fine tuning remain. In our case the potential is smooth and not discontinuous, and yet those two features persist.

While some can argue that a better choice of potential for recovering the infinite wall may get rid of the mass dependence and fine tuning, there are enough indications that that may have a different explanation. The standard and non-standard walls are mathematically valid and equally possible choices of boundary conditions. However as the name suggests the Dirichlet boundary conditions are the ones that are considered in physics in most cases. It has been pointed out that non-standard walls can also be physically interesting and yet they are much less used in physical applications. Perhaps the fine tuning is the explanation – to achieve Robin (or Neumann) boundary conditions the parameter must have a particular form. Such fine tuning is highly improbable to achieve in practice.

Finally let us point out that the method used here involves solving the star-eigenvalue equations for the generic Morse potential. Pure deformation quantization is notoriously difficult to achieve due to the pseudo-differential (or equivalently integro-differential) nature of the equations of motion. Few systems have been quantized in phase space quantum mechanics. In this sense a complete treatment of an integrable system contributes to the methods available for finding exact solutions in this framework. We solve the difference equations by using the Mellin transform, resulting in differential equations for the image. Then we transform the solution of the differential equation into a solution of the difference equation.

1.2 Deformation quantization and dissipation

Dissipative systems form a class of extreme systems that we can use to push the limits of deformation quantization. They are problematic to quantize in operator and path integral approaches so they are expected to be tricky in deformation quantization as well. Various techniques exist to treat dissipative systems. As an alternative approach phase space quantum mechanics should be able to provide a treatment in terms of a star product and phase space functions. On the other hand, one of the unique features of phase space quantum mechanics is the clear connection of the quantum with the classical physics. Dissipation can occur as a result of interaction with a large system or "environment", described classically or semi-classically. Also, as in the case of damped harmonic oscillator, the starting point is a classical equation of motion with classical Hamiltonian. Lastly the Wigner functions used as Wigner transforms of the density matrix, and other phase space distributions are already used in quantum optics and statistical mechanics when dissipation is present. The expectation is then that phase-space quantum mechanics, in which Wigner function is a central object, is a natural setting for the description of dissipation in quantum mechanics

A system that loses energy is viewed as a system interacting with a reservoir. The reservoir absorbs the energy that the system is dissipating forming together a closed system. Even though we are only interested in the evolution of the dissipative system we need to keep track of the reservoir degrees of freedom. This is well founded and very popular program with only one disadvantage. The reservoir is usually a big or/and complicated system that allows exact treatment only when simplifying conditions are assumed. For this reason in many cases effective approaches are used. What that means is that instead of introducing a reservoir, changes in the Hamiltonian and quantization procedure or the equations of motions are made. Some of the familiar features of the quantum mechanics of closed systems are abandoned. Quantum mechanics is a tightly woven structure and does not allow dissipation without modification. It can

involve one or more of the following: relaxing the reality/hermiticity condition on the Hamiltonian to include complex eigenvalues, modification of the canonical commutation relations, non-unitary evolution, modification of the equations of motion for the density matrix etc. These methods are justified as approximations, using first principles and they provide good qualitative and quantitative description with less technical complications.

Damped harmonic oscillator is perhaps the simplest possible example of a dissipation system. The approach we present in this thesis is an effective approach. Since the stress is on the deformation quantization aspect of the treatment perhaps many related physically interesting phenomena are omitted, the physical origin of the dissipation included. However this is not the purpose of this work. We show here that deformation quantization can be successfully applied and has the potential to contribute in ways different than those within the operator and path integral frameworks. Therefore applying phase space quantum mechanics is fruitful and more practical problems can eventually be solved within this program.

The results in this thesis are based on a method proposed by Dito and Turrubiates in [32]. They use a star product that is similar to but not the same as the Moyal star product. The new "star-gamma" product has an extra deformation parameter – the dissipation parameter for the damped harmonic oscillator. The starting point for their result is the classical equations of motion and the observation that if the Poisson bracket is modified we can write the equation of motions in phase space in Hamiltonian form. The system exhibits reasonable classical behaviour and the Hamiltonian remains unchanged. The dissipation is incorporated into the new Poisson bracket instead. Just as in the Moyal star product we exponentiate the bracket to define the new star-gamma product. With that product star-eigenvalue equations, Wigner functions and energies are found.

While the resemblance between the two cases – the Moyal product and the star-

gamma product are an obvious motivation for this method, one can ask why would that program work? Why does it make sense for us to write different star products for different physics? In phase space all products related through an invertible homomorphism are equivalent in some sense. Curiously enough this mathematical equivalence has nothing to do with physical equivalence. For example, if we use the Husimi probability distribution, which is a smoothed version of the Wigner function using a Gaussian weight, we are forced to change the star product. The new star product is mathematically equivalent to the Moyal star product, however it involves a coarse grained version of the Wigner function and the physics it describes. Therefore changing the star product to another will alter the physics even if we do not change the Hamiltonian of the system of interest and therefore it is a natural thing to do in the case of dissipation as well.

The Dito-Turrubiates method resembles some of the previously existing methods in certain ways. The homomorphism mentioned above transforms the simple harmonic oscillator to a complex Hamiltonian, resembling Dekker's Hamiltonian. Expanding in terms of the Moyal product and transforming with the Weyl map will produce a Lindblad-like master equation. The Wigner function resembles closely the symbol of the propagator for Caldirola-Kanai Hamiltonian etc. And yet it is not equivalent to any of the known treatments. This is to be expected since none of the effective treatments of the damped harmonic oscillator agrees completely with the rest. The Dito-Turrubiates method however proved to be different in some way and was clearly a nontrivial treatment.

Our contribution ([4]) amounts to resolving two serious issues with the original Dito-Turrubiates method. The first is the problem with the classical limit ($\hbar \to 0$). If the deformed star product is contracted (Planck's constant is taken to zero) it recovers the usual Poisson bracket. Physically it means that dissipation will disappear when the classical limit is taken. This of course is bad news since we quantized a classical

dissipation system and would like to recover the same system when the classical limit is taken. The second problem is even more obvious – if a Wigner function is taken to be real at some initial time, it inevitably acquires complex values over time. The dynamical evolution does not preserve the reality of the symbol of the density matrix and therefore it leads to complex populations.

To fix the problem we proposed a modification in the equations of motion. The change in form of the equations is subtle but fundamentally important. The new equations of motion allow the correct classical limit and at the same time preserve the reality of the Wigner function. The change was dictated by first principles and was motivated by a similar problem in operator quantum mechanics. Namely, the equations of motion for the density matrix have a commutator only because of the Hermiticity of the Hamiltonian, equivalently the star product commutator arises for the same reason. However, since the star-gamma is non-Hermitian the star-commutator use is not justified but assumed. Replacing it with the conjugate star product where necessary produces the correct limit and fixes the reality problem for the Wigner function.

1.3 Review of deformation quantization

Let as also mention that we provide here an overview of deformation quantization. It is usually outside of the scope of quantum mechanics textbooks and the interest towards it was renewed in the last ten years. Although the fundamentals have been known for a while, phase space quantum mechanics was not perceived as a completely independent quantization technique by most people. The merits of deformation quantization are numerous. It provides an unique insight into the relationship with classical physics, unmatched by the other quantization techniques. The language of phase space shared with classical mechanics allow both the similarities and the differences

to be shown in a way that is easy to understand and compare.

The physical quantities of the system in deformation quantization are conceptually the same as in the classical case. However the algebra of observables is deformed to a "quantum" one. The notion of state changes meaning – in classical mechanics it is simply a point in phase space, while in deformation quantization it is a quasi-probability distribution. While this demands a different interpretation of phase space in the quantum mechanical case, the transition from classical mechanics, through statistical physics into quantum mechanical understanding is smoother that in the standard quantization methods.

Deformation quantization is geometrical in spirit. Generally it deals with symplectic manifolds and the geometric structures existing on them. The existence of star products on every symplectic manifold has been shown, which allows for both generalizations and deeper understanding of certain features of *quantization* as a procedure.[3] More generally, we can have a system with a symmetry group (as in the case of spin). We can take the phase space to be a coadjoint orbit of the group with a symplectic structure naturally arising from the Lie group structure. The fact that deformation quantization is so geometrically transparent makes it a popular choice for generalizations, in string theory, for example. Also it satisfies the desire of some physicists for a justification of quantization coming from more geometrical arguments.

Some people argue that the strength of deformation quantization is its conceptual clarity and not in its calculational power. The reason is that the dynamical equations can be very complicated compared to the Schrödinger equation. However for mixed states where the systems are described by a density matrix instead of a wave function, the complexity of the equations in operator and deformation quantization is comparable since we have to solve master equations for an operator. Moreover, if the deformation quantization was the first method discovered one can argue that we

[3]More generally a classical system is described by a Poisson manifold. Loosely speaking, a Poisson manifold is just a manifold with Poisson brackets - later we will discuss in more detail.

would still have to solve the Schrödinger equation, since the underlying mathematical structure naturally leads to it (see section 2.7).

In many cases deformation quantization is no more difficult to work with, than standard quantum mechanics. In fact working with quasi-distributions instead of density operators is preferable in non-equilibrium statistical physics, quantum optics, etc. in many cases, even if we are not doing deformation quantization. The Wigner function, which is the deformation quantization counterpart of the wave function, can be (indirectly) measured in a lab, unlike operators, which makes it a natural choice even in operator quantum mechanics.

Deformation quantization can supplement the standard quantization techniques in both theoretical and experimental problems. In this thesis will emphasize the independence of this approach, developing it without any reference to the operator quantization or the path integral method, except to make a connection between them.

1.4 Summary

In the next *second chapter* of this thesis we present a comprehensive, application-oriented introduction to deformation quantization. To emphasize that this approach is independent of others we develop it from first principles and generalizations of classical mechanics and statistical physics. We provide a review of some of the most important topics, including fermionic particles. This last is largely ignored in introductory texts in the subject but its importance in theoretical and practical problems is clear.

In the *third chapter* we discuss contact interactions and the problems associated with them. We provide some essential background material and motivation behind our work. Then we consider the infinite wall as the prototypical contact interaction system, and also with bounded domain. We find that Robin boundary conditions for the infinite wall can be recovered as a limit of a mass dependent Morse potential for

certain choices of the parameters.

In the *fourth chapter* we expand the applicability of deformation quantization to dissipative systems. We start with a short introduction to a few methods used when dealing with dissipative systems. The idea we are trying to convey is that a system interacting with a reservoir can lose energy to the reservoir. However for practical calculations it is sometimes useful to use effective approaches, which do not keep track of the detailed evolution of all parts but instead use approximations and first principles to derive equations describing a dissipative system. We provide a solution to two problems in the original Dito-Turrubiates method – complex populations and an incorrect classical limit.

The last, *fifth chapter* is our conclusion. We discuss our results, expectations and questions that remain unanswered.

Chapter 2

Quantum mechanics in phase space

Quantum mechanics in phase space, also known as deformation quantization, is a quantization technique describing physical systems at microscopic scale. It is an alternative to the operator approach or path integral formalism that completely agrees with the observable world at the experimental level.

In this thesis we present deformation quantization from first principles. Some examples are worked out to better illustrate the theory. We point out the merits of the theory and try to convince you that deformation quantization is the quantum theory that best relates to its classical counterpart – showing relations between classical and quantum mechanics that seem obscure in any other approach. Deformation quantization is also a valuable tool for any physicist who needs quantum mechanics in their studies, supplementing the operator and path integral quantum mechanics in areas were last two are more complicated to use. Lastly, phase-space quantum mechanics is an autonomous formulation of quantum mechanics, independent of other approaches. It has been joked ([78]) that on another planet this could be the quantization technique that was discovered first.

The operator formalism is the first approach to encounter when studying quantum mechanics. Developed by Schrödinger, Heisenberg, Pauli, Dirac and others, it was

also the first to be discovered in the first quarter of the 20th century. It was a leap in thought and challenged our understanding of physics and broadened our view of the universe. Yet the ideas behind the quantum theory seemed very counter-intuitive to the physicist of the early 20th century and made many people, including Einstein, feel uncomfortable. The new operator "calculus" was a departure of the classical physics formalism which further amplified the difference between the two paradigms. The well understood and easy to imagine picture of the world described by differentiable functions on a phase space was forced away by operators, Hilbert spaces, eigenfunctions, probabilistic distributions and expectation values. Many people felt that the Hamiltonian formalism expressing so beautifully the laws of classical physics had rightfully found its place in quantum mechanics. On the other hand the phase space that is at the base of Hamiltonian mechanics did not play a role in the quantum theory. While remnants of the symmetry between coordinates and momenta could still be recognized in the freedom of choice between coordinate and momentum representation, the fact that you can choose one and completely ignore the other was regarded as a peculiarity of the formalism.

These were the factors that motivated the development of deformation quantization. In the 1920s Weyl found a correspondence relating functions on phase space and operators. Wigner discovered a quasi-distribution that allows the computation of probabilities using phase space integrals. These were the first indications that there may be a way of quantization that is true to the spirit of the classical theories. It was a step in the right direction however this was not a full-fledged theory since it relied on the standard quantum mechanics. The operator quantum mechanics was so successful that this work was mostly ignored, Wigner and Weyl actively involved in the development of the operator techniques themselves.

It was not until the late 40's when Grönewold and Moyal put phase-space quantum mechanics together. The fact that quantum mechanics deals with non-commuting

quantities was implemented in the new theory as a modified product between functions on phase space. Clearly the classical algebra of observables was not relevant anymore because it was incompatible with the Heisenberg principle. What Moyal and Grönewold realised is that that algebra needs to be deformed to a non-commutative one and the underlying algebraic structure should be related to the classical algebra in the limit when the deformation parameter goes to zero. This is how the star product was born – a non-commutative product in the algebra of the functions on phase space that mimicked the non-commutativity of the operator product. Later on it was shown that in some sense the star product is unique and exists for a sufficiently large class of phase spaces.

2.1 Hamiltonian mechanics

Let us begin with a brief overview of the features that make Hamiltonian formalism such an attractive approach to classical physics. Those same features have motivated physicists to pursue the development of a quantization technique that works in phase space in close analogy with statistical mechanics. We will also discuss states and observables as described in classical mechanics and statistical physics in relationship to possible generalizations, without venturing too deep into the mathematical formalism.

The Hamiltonian formalism provides an elegant formulation of classical mechanics that leads to deeper understanding of the underlying structures of the theory. In Hamiltonian mechanics a mechanical system means a system of particles with n degrees of freedom. Each particle's state is uniquely defined by its position and momentum, which are treated on an equal footing and therefore by a collection of points in a $2n$-dimensional space M called *phase space*. Those local coordinates

$$x = (q, p) = (q_1, ..., q_n, p_1, ..., p_n) \in M \tag{2.1}$$

allow a larger set of transformations to be considered. Hamiltonians assigned to different systems depend on the canonical variables and not on their derivatives, in contrast to the Lagrangian formalism, making the geometrical interpretation easier. Moreover the framework can be extended to other areas of physics: chaos theory, statistical mechanics, etc. and in particular provides a connection with quantum mechanics.

The Hamilton equations describing the evolution of the system

$$\dot{q} = \partial_p H(q,p), \quad \dot{p} = -\partial_q H(q,p)\,, \tag{2.2}$$

are first order. This allows phase portraits to be created thus allowing qualitative analysis of systems that cannot be integrated in closed form.

Let us denote the set of all possible states as Ω regardless of the approach we use. In classical mechanics[1] the set of all possible states will be the phase space or possibly a subset of it: $\Omega \subseteq M$. The evolution of a state will involve a succession of phase space coordinates which due to the equation of motion will constitute a partially smooth[2] curve – a *trajectory in phase space*. The possible irregularities will reflect the existence of contact interactions which will be our main concern in the next chapter.

Let $\mathcal{O}$ be the set of all physical observables. A natural assumption, made in classical mechanics, is that those observables depend on the state of the system at the time of the observation. Therefore an observable will be a one-parameter family, time being the parameter, of real smooth functions on the phase space M.

In order to allow algebraic manipulations with the observables, we need a product. For example, consider simple harmonic oscillator – the kinetic and potential energies require multiplication to be defined between the phase space coordinates. Typically

[1]From now on classical mechanics will always be considered to be described in Hamiltonian formalism.

[2]Smooth except for a finite number of points.

more complicated observables can be constructed from simpler ones. Therefore the observables form a subalgebra of the algebra of smooth functions $\mathcal{O} \subset (\mathcal{F}_{\mathbb{R}}(M), \cdot)$. In classical mechanics the algebraic operation is the usual commutative point-wise multiplication:

$$f, g \in \mathcal{F}_{\mathbb{R}}(M) \Rightarrow f \cdot g \in \mathcal{F}_{\mathbb{R}}(M)\,, \quad (f \cdot g)(x) = (g \cdot f)(x) \stackrel{\text{def}}{=} f(x)g(x)\,. \tag{2.3}$$

This is not the only possible structure in the space of smooth functions. The algebra of observables becomes a Lie algebra with the introduction of a Lie bracket – namely the Poisson bracket:

$$\{f, g\} = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right) . \tag{2.4}$$

Two other equivalent forms of the Poisson bracket are very commonly used in deformation quantization:

$$\{f, g\} \stackrel{\text{def}}{=} \sum_{i=1} f(\overleftarrow{\partial}_{q_i} \overrightarrow{\partial}_{p_i} - \overleftarrow{\partial}_{p_i} \overrightarrow{\partial}_{q_i}) g \stackrel{\text{def}}{=} P(f, g)\Big|_{\substack{q_1 = q_2 := q \\ p_1 = p_2 := p}} . \tag{2.5}$$

The first definition uses the arrows to indicate the direction in which the derivatives act, i.e. we are using the following notation:

$$f \overrightarrow{\partial}_q \, g \stackrel{\text{def}}{=} f \frac{\partial g}{\partial q} \quad \text{and} \quad f \overleftarrow{\partial}_q \, g \stackrel{\text{def}}{=} \frac{\partial f}{\partial q} g\,. \tag{2.6}$$

The second part of (2.5) uses a bi-differential operator defined as

$$P(f, g) = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_{1i}} \frac{\partial g}{\partial p_{2i}} - \frac{\partial f}{\partial p_{1i}} \frac{\partial g}{\partial q_{2i}} \right) f(q_1, p_1) g(q_2, p_2)\,. \tag{2.7}$$

Unlike in the operator approach, the Poisson bracket plays a very important role in deformation quantization, just like in classical mechanics. As we will discuss later, when exponentiated it generates a noncommutative product that is central to defor-

mation quantization.

The Hamiltonian $H(p,q)$ is an observable of special importance. For now we will only consider closed systems for which the Hamiltonian is an integral of motion and represents the energy of the system. Also it represents the system itself the sense that it generates the dynamical evolution of the physical observables :

$$\frac{df_t}{dt} = \frac{\partial f_t}{\partial t} + \{f_t, H\}, \qquad f_t = f(q(t), p(t); t)\,. \tag{2.8}$$

When the observables are the coordinates, imposing initial conditions is equivalent to picking a starting point for the trajectory in the phase space of the system. The equations along with the initial conditions determine completely the evolution of the system and any observables associated with it.

At any time τ measuring any value of a physical quantity f can be recovered by picking the appropriate representative from the family of phase space functions representing the physical quantity f_τ, identifying the point in phase $x = (q,p)$ space representing the state of the system and then evaluating the observable at that point of phase space, i.e. calculating $f_\tau(q,p)$.

Now let us turn our attention to systems that are too big to be practically possible to perform the program proposed or are statistical mixtures and we cannot describe the state in the way discussed earlier. For example, to describe a cup of tea, the number of measurement needed to specify a microstate is of order 10^{24}. A more practical approach would be the statistical mechanics program. A system can be in one of many microstates. Many of those will produce the same macroscopic quantities. Since it is practically impossible to determine the exact state of the system we associate a probability density that will weigh the possible outcomes:

$$\rho_{\rm cl}(q,p) \geq 0, \qquad \int_M \rho_{\rm cl}(q,p) d^n q\, d^n p = 1\,. \tag{2.9}$$

The equations of motion of the density distribution is the Liouville equation

$$\frac{\partial \rho_{\mathrm{cl}}}{\partial t} + \{\rho_{\mathrm{cl}}, H\} = 0\,. \tag{2.10}$$

In statistical mechanics the expectation value of a physical observable f can be expressed as a phase space integral weighed by the distribution (2.9)

$$\langle f \rangle = \int f(q,p)\rho_{\mathrm{cl}}(q,p) d^n q\, d^n p\,. \tag{2.11}$$

To include classical mechanics, we associate probability 1 to the state of the system and zero probability to all other possible states. Therefore it can be regarded as a special case when the probability distribution is a delta function centered at the point in phase space corresponding to the state of the system.

Only the average is fully deterministic and to particular microstates we can only associate probabilities:

$$(q,p) \mapsto \rho_{\mathrm{cl}}(q,p) d^n q\, d^n p\,. \tag{2.12}$$

For the ensemble interpretation and further information one can consult any of the numerous textbooks in statistical physics. However for our purposes this is enough since it points towards a possible generalization which will include quantum mechanical systems.

We can define a probability interpretation mapping that given an observable and a state associates a probability:

$$\mathcal{O} \times \Omega \to \mathcal{P}\,, \tag{2.13}$$

with $\mathcal{P}$ being the set of all infinitesimal probabilities as in (2.12). This will include all classical systems as long as we allow generalized functions to be probability distributions.

One can ignore the physical interpretation outlined above and think more abstractly of the system as specified by the probability distribution itself, leaving the phase space to play a more auxiliary role.

What happens when quantum phenomena are involved? Clearly we cannot apply the above program without modification. As we already argued phase space and phase space distributions have features that make them valuable and we would like them to be the core of the quantum theory. Since we no longer correctly describe the quantum world clearly the probability density is going to be different. Therefore the equations of motion will change for the quantum distribution. Also to accommodate the Heisenberg principle and the other noncommutative effects we will no longer be able to use the same algebra of observables since it is commutative. In particular the coordinates can no longer be measured together with arbitrary accuracy and therefore phase space will have a different interpretation, other that the space of all states. This and many more features will be discussed in the chapters to follow.

This line of thought clearly leads us to believe that someone with the skills and knowledge equal to that of an early twentieth century physicist would have had little trouble discovering quantum mechanics from generalization of classical physics. The leap of logic we need to make to generalize the theory is not as drastic as in the standard operator approach. We will show in this work that every aspect of deformation quantization follows naturally from first principles and generalizations. Deformation quantization can therefore be developed independently as a generalization of statistical physics. A feature of deformation quantization is that the relationship between classical and quantum mechanics is most transparent. Quantum mechanically the algebra of observables will be a deformation of the classical one and classical mechanics is a contraction of quantum mechanics.

2.2 Wigner-Weyl correspondence

Deformation quantization is an independent approach and can be developed from first principles as we will keep discussing. However the clearest way to introduce it is to use the standard operator quantum mechanics, since it is so familiar. Also it automatically provides the relationships between the alternative approaches, which helps to compare interpretations.

There is no quantization technique for which the transition from classical to quantum mechanics is unique. In the operator approach the operator expression corresponding to a physical quantity is determined by the order of the momentum and coordinate operators. In deformation quantization the symmetric *Weyl ordering* has a central role. To every monomial of q and p it gives a fully symmetrized polynomial of $\hat{q}$ and $\hat{p}$.

$$\mathcal{W}^{-1}(x) = \hat{x}, \;\; \mathcal{W}^{-1}(qp) = \frac{1}{2}(\hat{q}\hat{p} + \hat{p}\,\hat{q}), \;\; \mathcal{W}^{-1}(q^2p) = \frac{1}{3}\left(\hat{q}^2\hat{p} + \hat{q}\hat{p}\,\hat{q} + \hat{p}\,\hat{q}^2\right), \; ... \tag{2.14}$$

Using the binomial formula and (2.14) we can show that

$$\mathcal{W}^{-1}\left((aq + bp)^n\right) = (a\hat{q} + b\hat{p})^n\,, \tag{2.15}$$

i.e. the *Weyl map* of a binomial is equivalent to replacing the phase space coordinates with the corresponding operators: $q \to \hat{q}$, $p \to \hat{p}$. Now applying this to the Taylor expansion of the exponential function we arrive at:

$$\mathcal{W}^{-1}\left(\exp(aq + bp)\right) = \exp(a\hat{q} + b\hat{p})\,. \tag{2.16}$$

For any function we can write the Taylor expansion about $(0, 0)$ in the form $f(q, p) = f(\partial_a, \partial_b)\exp(aq + bp)\big|_{a=b=0}$ which can be used together with (2.16) to obtain the

general form of the Weyl map

$$\mathcal{W}^{-1}(f) = f(\partial_a, \partial_b) \exp(a\hat{q} + b\hat{p})\big|_{a=b=0} . \tag{2.17}$$

Different versions of that formula are often useful for different practical calculations. All of them can be derived using the same procedure as in (2.17):

$$\mathcal{W}^{-1}(f) = f(a,b) \exp(\overleftarrow{\partial}_a \, \hat{q} + \overleftarrow{\partial}_b \, \hat{p})\big|_{a=b=0} = \exp(\vec{\partial}_a \, \hat{q} + \vec{\partial}_b \, \hat{p}) f(a,b)\big|_{a=b=0} . \tag{2.18}$$

We can write an integral representation of the Weyl map using Fourier transform and its inverse in succession and applying (2.16) to the exponential factor:

$$\mathcal{W}^{-1}(f) = \frac{1}{(2\pi)^2} \int d\tau \, d\sigma \, dq \, dp \, f(q,p) \exp[i\tau(\hat{p} - p) + i\sigma(\hat{q} - q)] . \tag{2.19}$$

We have been using $\mathcal{W}^{-1}$ implying that the Weyl map is the inverse of another map. Indeed the *Wigner transform* $\mathcal{W}$ will take an operator (involving $\hat{x}$ and $\hat{p}$) and will return a phase space function. In defines a map from the quantum observable to the classical ones:

$$\mathcal{W}(\hat{f}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dy \, e^{-ipy} \langle q + \hbar y/2 | \hat{f} | q - \hbar y/2 \rangle . \tag{2.20}$$

The image $f = \mathcal{W}(\hat{f})$ of an operator is called the *symbol* of that operator. A more general expression that does not rely on a particular basis is given by

$$f(q,p) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} d\xi \, d\eta \, \mathrm{Tr}\left[\hat{f} \, e^{-i(\xi\hat{q} + \eta\hat{p})}\right] e^{i\xi q + i\eta p} . \tag{2.21}$$

This form is important, because it allows us to write the Wigner transform as a trace of two operators

$$f = \mathrm{Tr}(\hat{f}\hat{w}) . \tag{2.22}$$

This form allows generalizations to be made for curved symplectic manifolds, and in particular, for particles with spin. The operator $\hat{w}$ is called *quantizer* and in the case when $\mathbb{R}^{2n}$ is our phase space it is simply

$$\hat{w} = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} d\xi \, d\eta \, e^{i\xi(q-\hat{q})+i\eta(p-\hat{p})} \, . \tag{2.23}$$

The Wigner-Weyl correspondence relates classical quantities to quantum ones. Functions on phase space correspond to operators involving $\hat{q}$ and $\hat{p}$. The observables on phase space commute, while the operators do not. Therefore we need to construct a non-commutative algebra of observables on phase space, similar to the operator algebra.

2.3 Moyal product

Let us consider a product of two Weyl-ordered operators, for example $\hat{q}$ and $\hat{p}$. By definition those are Weyl-ordered operators. However their product $\hat{q}\hat{p}$ is not. More generally – when is the product of two Weyl-ordered operators another Weyl-ordered operator? Using (2.19) we write

$$\hat{f}\hat{g} \propto \int d\tau_1 d\sigma_1 d\tau_2 d\sigma_2 dx_1 dx_2 \, f(x_1) g(x_2) e^{i\tau_1(\hat{p}-p_1)+i\sigma(\hat{q}-q_1)} e^{i\tau_2(\hat{p}-p_2)+i\sigma_2(\hat{q}-q_2)} \, , \tag{2.24}$$

where $x = (q, p)$ and $dx = dq\, dp$. We can rearrange the terms in the exponential and change the variables in order to isolate an exponential as in (2.19). What is left will be the symbol of $\hat{f}\hat{g}$. The substitution

$$\tau_1 = \tau - 2(q-q_1)/\hbar \, , \quad \tau_2 = 2(q-q_1)/\hbar \, , \quad \sigma_1 = \sigma + 2(p-p_1)/\hbar \, , \quad \sigma_2 = -2(p-p_1)/\hbar \tag{2.25}$$

leads to an expression identical to (2.19)

$$\hat{f}\hat{g} = \frac{1}{(2\pi)^2}\int d\tau\, d\sigma\, dq\, dp\ (f*g)(q,p)\exp[i\tau(\hat{p}-p)+i\sigma(\hat{q}-q)]\,, \tag{2.26}$$

if we define $(f*g)(q,p)$ to be the integral

$$(f*g)(x) = \int \frac{dx_1 dx_2}{\pi^2\hbar^2} f(x_1)g(x_2)e^{-\frac{2i}{\hbar}[p(q_1-q_2)+p_1(q_2-q)+p_2(q-q_1)]}\ . \tag{2.27}$$

Therefore if we define a special multiplication operation for symbols of operators, that product will transform into the product of the corresponding operators.

This result is due to Grönewold. He showed that a non-commutative product exists in the algebra of classical observables – the *Grönewold-Moyal star product* (or more commonly as the *Moyal star product*) . It can be written in terms of derivatives

$$f*g = f(q,p)\exp\left\{\frac{i\hbar}{2}\left(\overleftarrow{\partial}_q\overrightarrow{\partial}_p - \overleftarrow{\partial}_p\overrightarrow{\partial}_q\right)\right\}g(q,p)\,. \tag{2.28}$$

It mimics the operator product in a sense we will explain below (we will also show the equivalence between the two definitions). As before the arrows imply that $\overleftarrow{\partial}$ is a derivative acting to the left and ignoring the argument to the right, similarly $\overrightarrow{\partial}$ acts to the right only. Under the Moyal star product the observables in phase space form a noncommutative algebra. Remarkably, the Grönewold's result leads to a much stronger statement:

$$\mathcal{W}^{-1}(f)\ \mathcal{W}^{-1}(g) = \mathcal{W}^{-1}(f*g)\,. \tag{2.29}$$

This is easy to see when we apply the first version of the Weyl map (2.18) to f and the second to g and apply the Baker-Campbell-Hausdorff formula $e^A e^b = e^{[A,B]/2}e^{A+B}$ to the result:

$$\mathcal{W}^{-1}(f)\ \mathcal{W}^{-1}(g) = f(a_1,b_1)e^{\overleftarrow{\partial}_{a_1}\hat{q}+\overleftarrow{\partial}_{b_1}\hat{p}}\ e^{\overrightarrow{\partial}_{a_2}\hat{q}+\overrightarrow{\partial}_{b_2}\hat{p}}g(a_2,b_2)\big|_{a_i=b_i=0}$$

$$= e^{(\partial_{a_1}+\partial_{a_2})\hat{q}+(\partial_{b_1}+\partial_{b_1})\hat{p}} f(a_1,b_1) e^{\frac{i\hbar}{2}(\overleftarrow{\partial}_{a_1}\vec{\partial}_{b_2}-\overleftarrow{\partial}_{b_1}\vec{\partial}_{a_2})} g(a_2,b_2)\big|_{a_i=b_i=0}$$
$$= e^{(\partial_a\hat{q}+\partial_b\hat{p})} f(a,b) e^{\overleftarrow{\partial}_a\vec{\partial}_b-\overleftarrow{\partial}_b\vec{\partial}_a} g(a,b)\big|_{a=b=0} = \mathcal{W}^{-1}(f*g)\,.$$

The star product along with the Wigner-Weyl correspondence define a homomorphism between the algebras of classical and quantum observables. Physically that means that in the well-known operator quantum mechanics, multiplication of two observables is equivalent to a multiplication of the corresponding phase space functions (symbols) using the star product and then transforming with the Weyl map. Consequently we don't need to use operators – instead we can use the phase space functions and a star product. Let us recall that a non-commutative algebra already exists in the space of phase space functions – the Lie algebra defined by the Poisson bracket. These two noncommutative algebras are closely related. We will develop these ideas extensively in the later sections.

Now let us go back to the star product. The exponential in (2.28) is understood as a series. It is a pseudodifferential operator which can be seen if we expand the exponential and apply the differential operators.

$$(f*g)(q,p) = \sum_{m,n=0}^{\infty} \left(\frac{i\hbar}{2}\right)^{m+n} \frac{(-1)^m}{m!\,n!}\, \partial_p^m \partial_q^n f(q,p)\, \partial_p^n \partial_q^m g(q,p)\,. \tag{2.30}$$

The star product can also be written in a different form that is very useful for calculations and emphasizes the relationship with the Poisson bracket. The $*$-product is a formal series involving powers of the Poisson bracket (2.5):

$$(f*g)(q,p) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i\hbar}{2}\right)^n P^n(f(x_1),g(x_2))\Big|_{\substack{p_1=p_2=p\\ q_1=q_2=q}}\,, \tag{2.31}$$

Using the notation in (2.7). This has a profound significance – the Moyal product is an exponentiation of the Poisson bracket. The mathematical structure that governs the classical physics is continued to a new mathematical structure in the algebra of

quantum quantities. The star product is a deformation of the classical commutative product with a deformation parameter equal to the Planck's constant. Indeed if we take Planck's constant to approach zero then it will recover the usual product of two phase space functions.[3]

The $*$-product can also be written using so-called Bopp shifts, simply by using the Taylor series. This is very convenient for practical computations as long as f has a simple form:

$$(f * g)(q,p) = f\left(q + \frac{i\hbar}{2}\,\vec{\partial}_p, p - \frac{i\hbar}{2}\,\vec{\partial}_q\right) g(q,p)\,. \tag{2.32}$$

We use this representation extensively, for example in the treatment of a linear potential as well as for the simple harmonic oscillator.

Finally, let us point out that the Moyal $*$-product has the property

$$\overline{f * g} = \bar{g} * \bar{f}\,. \tag{2.33}$$

We say that the star product is *Hermitian* since clearly this property reflects the operator identity $(\hat{f}\hat{g})^\dagger = \hat{g}^\dagger \hat{f}^\dagger$.

All these pseudo-differential representations, in general, involve infinitely many derivatives which implies that the product is non-local. This can be made explicit if we use an integral representation of the Moyal $*$-product.

Integral representation of the star product

For many purposes the integral definition is very useful. The integral representations are helpful to make a connection to the path integral approach, e.g. see [58]. It is

[3]Strictly speaking, the Planck's constant is divided by a variable with matching dimensions and that variable is taken to infinity so that there is no confusion with the constant status of $\hbar$. We will always talk as if the Planck's constant can be varied with a word of caution in the back of our minds.

also used in practical calculations involving exponential functions. Most importantly, the integral representation does not demand differentiability but integrability. This can come in handy when discontinuous, sharp potentials are involved.

Let us define a *symplectic product* in the phase space[4]:

$$x_1 \wedge x_2 = \sum_i (\partial_{q_{1,i}} \partial_{p_{2,i}} - \partial_{p_{1,i}} \partial_{q_{2,i}}) \,. \tag{2.34}$$

Now we can show that the differential and the integral definition are equivalent:

$$\begin{aligned} (f * g)(q,p) = \exp\left\{ -\frac{i\hbar}{2} \partial_{x_1} \wedge \partial_{x_2} \right\} \big(f(x_1) g(x_2) \big) \Big|_{\substack{p_1=p_2=p \\ q_1=q_2=q}} = \\ \int dx' dx'' \left\{ e^{-\frac{i\hbar}{2} \partial_{x_1} \wedge \partial_{x_2}} f(x_1) g(x_2) \right\} \delta(x' - x) \delta(x'' - x) \,. \end{aligned} \tag{2.35}$$

We use the Fourier transforms of the functions

$$f(q,p) = \int_{-\infty}^{+\infty} e^{i\sigma x + i\tau p} \tilde{f}(\tau, \sigma) d\tau d\sigma \tag{2.36}$$

and the inverse Fourier transform

$$\tilde{f}(\sigma, \tau) = \int_{-\infty}^{+\infty} e^{-i\sigma x' - i\tau p'} f(x', p') dx' dp' \tag{2.37}$$

and perform all the integration over the primed variables to obtain

$$(f * g)(x) = \int \frac{dx_1 dx_2}{\pi^2 \hbar^2} f(x_1) g(x_2) e^{-\frac{2i}{\hbar}[p(q_1 - q_2) + p_1(q_2 - q) + p_2(q - q_1)]} \,, \tag{2.38}$$

which is exactly the expression (2.27) for the star product.

[4]The product can be generalized to include symplectic manifolds other than $\mathbb{R}^{2n}$. The product then has the form $x \wedge y = (\omega^{-1})^{ij} x_i y_j$ where ω^{-1} is the inverse of the symplectic form.

The noncommutativity is explicit if we rewrite our integral as

$$(f * g)(q,p) = \int \frac{dudvdwdz}{\pi^2\hbar^2} f(q+u,p+v)g(q+w,p+z)\exp\left[\frac{2i}{\hbar}(uz-vw)\right] \quad (2.39)$$

since in this form the asymmetry in the arguments is apparent. For example one can calculate the Heisenberg canonical commutation relation:

$$x * p - p * x = i\hbar\,. \quad (2.40)$$

One can give a certain geometric interpretation of the star product. The integral is weighted by the exponentiated symplectic area of the triangle spanned by the origin, $x - x_1$ and $x - x_2$

$$(f * g)(\vec{x}) = \int \frac{d\vec{x}_1 d\vec{x}_2}{\pi^2\hbar^2} f(\vec{x}_1)g(\vec{x}_2)\exp\left[\frac{4i}{\hbar}A\left(\vec{x},\vec{x}_1,\vec{x}_2\right)\right]\,. \quad (2.41)$$

2.4 The Wigner function

The Wigner function can be introduced as a quasi-probability distribution that gives the measure on the phase space. However a great deal can be learned if we exploit the numerous relationships with the operator approach. Both points of view are beneficial to the understanding of the Wigner function so they will be presented. The easiest way is, again, coming from standard operator quantum mechanics.

Let us assume that whatever system we are interested in has Hamiltonian $\hat{H}$. It is described by a known wave function $\Psi(x,t)$ that we found solving the Schrödinger equation $\hat{H}\Psi = i\hbar\partial_t\Psi$. The Wigner function is defined as

$$\rho(q,p;t) = \int \frac{dy}{2\pi} e^{-ipy}\Psi^*\left(q - \frac{\hbar y}{2}, t\right)\Psi\left(q + \frac{\hbar y}{2}, t\right)\,, \quad (2.42)$$

where the case of a 2-dimensional phase space is considered for simplicity. For now we consider stationary Wigner functions. We treat the time dependence in a later section.

The Wigner function has a central role in deformation quantization. Conceptually it will replace the wave function, or more generally the density matrix as means to define the state of a quantum system. We will now discuss its properties.

Let us start with an example: the simple harmonic oscillator ($m = \omega = 1$). The Wigner function for the ground and first excited states can be found using Gaussian integral:

$$\rho_0(q,p) = \frac{1}{\sqrt{\pi\hbar}} \int \frac{dy}{2\pi} e^{-ipy} e^{-\frac{1}{2}(q-\hbar y/2)^2} e^{-\frac{1}{2}(q+\hbar y/2)^2} = \frac{1}{\pi\hbar} e^{-\frac{1}{\hbar}(p^2+q^2)} \,. \tag{2.43}$$

Similarly after integration by parts we can find the Wigner function corresponding to the first excited state:

$$\rho_1(q,p) = -\frac{2}{\pi\hbar^2} \left(p^2 + q^2 - \hbar/2\right) e^{-\frac{1}{\hbar}(p^2+q^2)} \,. \tag{2.44}$$

The ground state is a non-negative integrable phase space function and it can be normalized, i.e. it defines a probability distribution. However the first, and in fact all other excited states, can assume negative values. This example shows us the feature that physicists mistook for a serious shortcoming – its negative values. A probability distribution is Lebesgue integrable (ours are more or less obviously such) non-negative function, i.e. $\rho(q,p) \geq 0$. The Wigner distribution is therefore not a probability distribution. However it encodes the right physics as we will keep convincing ourselves. For that reason we will call it a *quasi-probability* distribution.

The negative parts of the Wigner function are fundamentally important since it will lead to the Heisenberg principle. It is not a disadvantage of the theory - on the contrary quantum effects will not be described correctly in this formalism without this

feature. Also Wigner function is not observable directly, much like the wave function. Instead we can construct coordinate space "shadow" that is indeed a probability distribution in the coordinate space. Let us consider a pure state with energy E_n[5]

$$\frac{1}{2\pi\hbar}\int dp\,\rho_n(q,p) = \frac{1}{2\pi\hbar}\int e^{-i\xi p/\hbar} d\xi dp \langle q+\xi/2|n\rangle\langle n|q-\xi/2\rangle \qquad (2.45)$$
$$= \langle q|n\rangle\langle n|q\rangle = |\psi_n(q)|^2\,.$$

In a similar way we can find the momentum shadow integrating the alternative definition of Wigner function (q and p switched)

$$\frac{1}{2\pi\hbar}\int dx\,\rho_n(q,p) = \langle p|n\rangle\langle n|p\rangle = |\tilde{\psi}_n(p)|^2\,. \qquad (2.46)$$

Therefore the projections are true probability distribution in the coordinate and momentum space spaces. They provide us with measures in the coordinate and momentum space. Therefore the q- and p-projections, or marginal probability distributions,

$$\mathbb{P}\{a\le q\le b\} = \int_a^b dq \int dp\ \rho(q,p),\ \mathbb{P}\{\alpha\le p\le\beta\} = \int_\alpha^\beta dp \int dq\ \rho(q,p) \qquad (2.47)$$

have the form from statistical mechanics, using phase space integrals, and yet recover the familiar results of operator quantum mechanics.

So far we have worked with the wave function, i.e. with pure states. In operator quantum mechanics the mixed states are treated in terms of the density operator. Recall that the density operator is used instead of the wave function when there is entanglement or our knowledge of the system is limited or statistical in nature. The wave function formalism is not sufficient to describe some phenomena that are physically interesting. This includes dissipation which will be of interest to us in the last chapter, where we consider a subsystem interacting with a larger system

[5]Later we will show the probabilistic interpretation of the general Wigner function.

or a reservoir. However the size of the system is not that important even for the case of two particle system we need to use density operator if we treat one of the particles as a system of interest only. To introduce the density operator is quite natural. Let us consider two systems A and B with their corresponding Hilbert spaces $\mathcal{H}_\alpha = \text{span}\{|i\rangle_\alpha | \alpha \in I_\alpha\}$, where $\alpha = A, B$ and I is some indexing interval. In the case when the two systems are interacting we can write the Hilbert space as $\mathcal{H}_A \otimes \mathcal{H}_B$ and any pure state will then be written as:

$$|\psi\rangle_{AB} = \sum_{i,j} C_{ij} |i\rangle_A \otimes |j\rangle_B \,. \tag{2.48}$$

The density matrix of the system of interest A is obtained by a partial trace over the system B from the density operator for the pure state of the entire system $\rho_{AB} = |\psi\rangle_{AB}\langle\psi|_{AB}$[6]

$$\hat{\rho}_A = \text{Tr}_\text{B}(|\psi\rangle_{AB}\langle\psi|_{AB}) = \sum_{i,j;k} C_{ik}\bar{C}_{jk} |i\rangle_A \langle j|_A \,. \tag{2.49}$$

Choosing a basis in which the density operator is diagonal we can write it in the form:

$$\hat{\rho}_A = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|, \quad 0 \leq p_\alpha \leq 1. \quad \sum_\alpha p_\alpha = 1 \,. \tag{2.50}$$

The density operator therefore can be interpreted as describing an incoherent mixture of possible pure states with additional weight coming from probabilities. In other word we can see it as ensemble of states which the system can assume with certain probabilities. This means that the relative phases cannot be found experimentally. These probabilities are due to the system B and unlike the probabilities associated with pure states. This means that naturally in deformation quantization mixed states

[6]More generally we can prepare a statistical mixture of pure states. This will also require a density matrix, however it does not necessarily arise as a partial trace. Since we recover the form (2.50) in both cases, it will not affect the definition of the Wigner function.

will be represented by Wigner transform (2.21) of the general density operator:

$$\rho \stackrel{\text{def}}{=} \frac{\mathcal{W}(\hat{\rho})}{2\pi\hbar}\,. \tag{2.51}$$

This definition would not have been available if deformation quantization was the first approach discovered. The Wigner function would simply come as a generalization of the classical density. Bear in mind though, that after postulating the physical requirements and the corresponding equations from first principles and generalizations of the classical theory we would not have to relate to the operator approach to describe physics. Here it is done so that the transition is in the more familiar language of operator quantum mechanics.

2.5 Moyal equation. Mean value and Ehrenfest theorem. The Heisenberg principle.

Here we discuss the generalizations that lead to the dynamical equation of motion for the Wigner function – the Moyal equation. Also we discuss features of the theory that connect deformation quantization to classical mechanics, as well as the differences. We will see how known phenomena like the Ehrenfest theorem and the Heisenberg principle bring new interpretation to phase space and relationship between classical physics and deformation quantization.

The Moyal equation

Knowing the Wigner function can tell us everything about the system, but how do we find it for a given Hamiltonian? Let us recall that the Wigner function is the Wigner

transform of the density operator. Now consider that the density operator satisfies

$$i\hbar\frac{\partial\hat{\rho}}{\partial t} + [\hat{\rho}, \hat{H}] = 0\,. \tag{2.52}$$

A straightforward application of the Wigner transform on the above equation will produces the dynamical equation for the time dependent Wigner function:

$$i\hbar\frac{\partial\rho}{\partial t} + [\rho, H]_* \stackrel{\text{def}}{=} i\hbar\mathcal{L}\rho = 0\,, \tag{2.53}$$

where $[f, g]_* \stackrel{\text{def}}{=} f * g - g * f$ is known as the *Moyal bracket*. The above equation (2.53) is called *Moyal equation* and it plays a central role in deformation quantization. Its significance is the same as the time-dependent Schrödinger equation for operator quantum mechanics. Using (2.53) we can determine the evolution of the system without the need for computing the wave functions or density matrix first.

A significant point is that the equation can be simply postulated just as the Schrödinger equation is postulated in operator quantum mechanics. We already know that the observables will satisfy a $\hbar$-corrected algebra and we know that the probability distribution describing a classical system will be generalized to a quasi-probability distribution in the quantum case. The Moyal equation simply comes as a generalization of its classical counterpart. The form of the equation is remarkably similar to the Liouville theorem for the classical phase space density:

$$\frac{\partial\rho_c}{\partial t} + \{\rho_c, H\} = 0\,. \tag{2.54}$$

In fact this is by far the most obvious and conceptually clear transition from classical equations of motion to quantum equations of motion. The quantization scheme

$$\{f, g\} \to \frac{1}{i\hbar}\,[f, g]_* \tag{2.55}$$

can be directly applied to the classical equation of motion without any modification, as a direct generalization from classical and statistical mechanics.

Average value. Ehrenfest theorem. Phase-space interpretation

Expectation values in deformation quantization are calculated as phase space integrals:

$$\langle f \rangle = \int dqdp f(q,p)\rho(q,p)\,. \tag{2.56}$$

In fact this is one of the primary motivations for deformation quantization. An average must be a phase space integral with a measure that is determined in the spirit of statistical mechanics. In an independent approach this would have been postulated as a generalization of statistical mechanics.

Let us show that the definition (2.56) is equivalent to the one given in standard quantum mechanics as long as we use Wigner functions as defined by (2.51). In general we can write the average as weighted sum over all possible values

$$\langle f \rangle = \sum_n P_n f_n\,, \tag{2.57}$$

with the probabilities P_n being the weights. In operator quantum mechanics we can write them, in the case of pure states, as $P_n = |\langle n|\psi\rangle|^2$ – the probability to find the particle in a state for which f assumes value f_n. Note that (2.57) does not depend on the fact that the physical values of f are represented here by the eigenvalues of an operator.

We will now provide the relationship between the two approaches. For a mixed state, provided we use a basis in which the density matrix is diagonal we have an incoherent mixture of states:

$$\rho = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha| \tag{2.58}$$

we have probabilities associated with the possible pure states $|\psi_\alpha\rangle\langle\psi_\alpha|$. This leads to the well known trace formula for mixed states:

$$\langle f\rangle = \sum_\alpha p_\alpha \langle\psi_\alpha|\hat{f}|\psi_\alpha\rangle = \mathrm{Tr}(\hat{\rho}\hat{f})\,. \tag{2.59}$$

Both formulations are consistent and give the same result. Using the Wigner-Weyl correspondence and the trace formula (2.59) we can easily see that:

$$\begin{aligned}\langle f\rangle &= \int dq\,dp f(q,p)\rho(q,p) = \\ &\int dx\,dy\,dz\,e^{-ipy}\,\langle q+\hbar y/2|\,\hat{f}\,|q-\hbar y/2\rangle\,e^{-ipz}\,\langle q+\hbar z/2|\,\hat{\rho}\,|q-\hbar z/2\rangle = \\ &\int d\xi\,d\eta\,\langle\xi|\,\hat{f}\,|\eta\rangle\,\langle\eta|\,\hat{\rho}\,|\xi\rangle = \mathrm{Tr}(\hat{\rho}\hat{f})\,.\end{aligned} \tag{2.60}$$

The cyclic property of the trace has its equivalent in phase space:

$$\int dx f(x) * g(x) = \int dx\, g(x) * f(x) = \int dx f(x) g(x)\,. \tag{2.61}$$

This is easy to see since the surface terms are integrated out for all physical observables.

With this as a prerequisite we can explore the equivalent of the Ehrenfest theorem and the consequences in phase space. The evolution of the mean value of a function that does not have an explicit time dependence is given by

$$i\hbar\frac{d\langle f\rangle}{dt} = i\hbar\int dx\frac{\partial\rho}{\partial t} * f = \int dx\,[H,\rho]_* * f = \int dx\rho\,[f,H]_* = \langle[f,H]_*\rangle \tag{2.62}$$

by the virtue of the cyclic property (2.61) we then have "Heisenberg equation" for the physical quantity:

$$i\hbar\frac{df}{dt} = [f,H]_*\,. \tag{2.63}$$

Clearly this is a Wigner-Weyl transform of the operator version.

However there a few features that are unique to the deformation quantization. Deformation quantization provides corrections to the classical motion that depend on the Planck's constant:

$$i\hbar\frac{df}{dt} = \{f, H\} + (...)\hbar + (...)\hbar^2 + \mathcal{O}(\hbar^3)\,, \tag{2.64}$$

where the ellipses in the brackets stand for expressions depending on derivatives of f and H only. Moreover classical mechanics tells us that the classical probability flows like an incompressible fluid according to the Liouville equation:

$$\frac{d\rho_{\rm cl}}{dt} = \frac{\partial\rho_{\rm cl}}{\partial t} + \dot{q}\frac{\partial\rho_{\rm cl}}{\partial q} + \dot{p}\frac{\partial\rho_{\rm cl}}{\partial p} = 0\,. \tag{2.65}$$

That can no longer be said in the quantum case in quantum mechanics. For some region V we want to see how the probability will change in time:

$$\frac{d}{dt}\int_V dx\,dp\;\rho(q,p) = \int_V dx\,dp\left(\frac{1}{i\hbar}[H,\rho]_* - \{H,\rho\}\right) \neq 0\,. \tag{2.66}$$

The last expression can be zero if V is the whole phase space but in general is nonzero. Therefore the probability of the particle being in a certain region of phase space will change.

Wigner trajectories

The analogy with classical mechanics can be pushed further in some cases – we can define trajectories in deformation quantization as in classical mechanics. To see that, let us consider the Moyal equation explicitly, written for a few terms only:

$$\frac{\partial\rho}{\partial t} = -\frac{p}{m}\;\frac{\partial\rho}{\partial q} + \frac{\partial V}{\partial q}\;\frac{\partial\rho}{\partial p} + \mathcal{O}(\hbar)\,. \tag{2.67}$$

Clearly in the case when $V(q)$ is at most a quadratic polynomial, as in free particle and simple harmonic oscillator, the $\mathcal{O}(\hbar)$ term is identically zero. Equation (2.67) is in fact classical. Moreover, it implies that the dynamical equations for the phase space coordinates are the Hamiltonian equations, even for the quantum case:

$$\dot{q} = p/m, \quad \dot{p} = -\partial_q V(q)\,. \tag{2.68}$$

In fact the last is true for every Hamiltonian that can be written as $H = p^2/2m + V(q)$ since the evolution of the phase space coordinates according to (2.63) is simply:

$$\dot{q} = [q, H]_* = -\partial_p H, \quad \dot{p} = [p, H]_* = -\partial_q H\,, \tag{2.69}$$

which is identical to (2.68). In other words deformation quantization and classical mechanics are exactly the same as far as the evolution of the phase space coordinates is concerned. However in classical mechanics these equations determine the state since the phase space is space of states and in deformation quantization that is not the case. Therefore the interpretation is very different.

Let us consider a general potential (not linear or quadratic). We can write the equation of motion (2.67) in the form of classical equation

$$\frac{\partial \rho}{\partial t} = -\frac{p}{m}\frac{\partial \rho}{\partial q} + \frac{\partial V_{\text{eff}}(q)}{\partial q}\frac{\partial \rho}{\partial p}\,. \tag{2.70}$$

Here however the $*$-product does not terminate and we need to define an effective potential $V_{\text{eff}}(q)$ in order to achieve (2.70). Comparing with the Moyal equation the effective potential must satisfy

$$\partial_q V_{\text{eff}}(q)\partial_p \rho = \sum_{n=0}^{\infty} \left(\frac{\hbar}{2i}\right)^{2n} \frac{\partial^{2n+1} V_{\text{eff}}(q)}{\partial q^{2n+1}} \frac{\partial^{2n+1} \rho}{\partial p^{2n+1}}\,. \tag{2.71}$$

Using the new potential we can write the equations of motion of the phase space coordinates in terms of the new effective potential just as before

$$\dot{q} = p/m, \quad \dot{p} = -\partial_q V_{\text{eff}}(q)\,. \tag{2.72}$$

The Wigner function now satisfies the equation of motion trivially just like in the quadratic case. The curves defined by the above equations are called *Wigner trajectories* and are the generalization in the case of quantum systems.

Is that not a contradiction with the common lore? To answer that let us notice that (2.71) involves the Wigner function. In fact we need to solve simultaneously for the Wigner function and the effective potential. In other words this method will not provide any simplification in general. Moreover effective potential may not even exist for generic $V(q)$ and thus Wigner trajectories will not exist either, reconciling deformation quantization with standard quantum mechanics.

However in the case of semi-classical systems we can write a zeroth order approximation of the Wigner function. Using approximation techniques one can find both $\rho(q,p,t)$ and V_{eff} making it possible for the Wigner trajectories to be found using (2.72). The trajectories will make sense now but only as much as the Bohr orbits do in relation to the hydrogen atom.

The Heisenberg principle

The Heisenberg principle is one of the cornerstones in quantum mechanics. Let us now derive it for deformation quantization and discuss its implications.

A star-square $f * f$ does not have a positive average, unless f is real. Instead we can write $\langle f * \bar{f} \rangle \geq 0$. Let us now choose the function appropriately, as in [78], i.e. to be a first order polynomial in the phase space coordinates

$$g(q,p) = a + bq + cp\,. \tag{2.73}$$

Expanding the expression $\langle g * \bar{g} \rangle$ in terms of the arbitrary constants a, b and c we get a bi-linear form

$$a\bar{a} + b\bar{b}\langle q * \bar{q} \rangle + c\bar{c}\langle p * \bar{p} \rangle + (\bar{a}b + \bar{b}a)\langle q \rangle + (\bar{a}c + \bar{c}a)\langle p \rangle \tag{2.74}$$

$$+\bar{c}b\langle p * q \rangle + \bar{b}c\langle q * p \rangle \geq 0\,. \tag{2.75}$$

That is positive semi-definite. According to the Sylvester's criterion the matrix of this bi-linear form

$$\begin{pmatrix} 1 & \langle q \rangle & \langle p \rangle \\ \langle q \rangle & \langle q * q \rangle & \langle p * q \rangle \\ \langle p \rangle & \langle q * p \rangle & \langle p * p \rangle \end{pmatrix} \tag{2.76}$$

will have non-negative leading principal minors. In particular that is true for the determinant to be non-negative. Defining the variances in the usual way

$$(\Delta q)^2 = \langle (q - \langle q \rangle)^2 \rangle, \quad (\Delta p)^2 = \langle (p - \langle p \rangle)^2 \rangle \tag{2.77}$$

and evaluating the $*$-products in (2.76) leads to the inequality

$$(\Delta q)^2 (\Delta p)^2 \geq \frac{\hbar^2}{4} + \Big(\langle (q - \langle q \rangle)(p - \langle p \rangle) \rangle \Big)^2. \tag{2.78}$$

The Heisenberg principle is a direct consequence of the above.

The fact that the momentum and the position cannot be measured with infinite accuracy simultaneously means that points of phase space cannot be identified. While in statistical mechanics points in phase space have the meaning of states (with associated probabilities) in deformation quantization such interpretation is impossible. However we can still think of the states of the system as the probability distributions associated to them, as mentioned in the first section.

2.6 Star products. C-equivalence

The Moyal product is not the only star product that one can construct given a particular phase space. Here we will discuss different star products on $\mathbb{R}^n$ and how they are related.

Let us recap. Quantization will be considered a procedure which takes a classical system and produces a quantum system. In the Hamiltonian formalism a phase space with Poisson bracket, a Poisson manifold, will represent the possible states that the system can assume. The most prominent difference between that and the quantum mechanics is the existence of the Heisenberg uncertainty principle. The implications of it are tremendous: as the coordinate and the momentum are no longer measurable simultaneously the concept of the phase space as a space of states is no longer sensible. In quantum mechanics states cannot be represented as points in the phase space! The quantum algebra of observables is no longer commutative. The multiplication of the algebra of observables has to be changed in a transition from classical to quantum mechanics. More generally we want the quantum observable to be smooth functions on a phase space or Poisson manifold. To account for the quantum behaviour of the system we introduce an abstract product in the algebra of the observable – the *star product*.

Physical properties (postulates) that an abstract star product must obey are listed below.

1. In the classical limit the star product needs to recover the pointwise multiplication.

$$\lim_{\hbar \to 0} f * g = fg \,. \tag{2.79}$$

2. The dynamics of the system in the case of the Moyal product is given by the star-commutator while classically it is given by the Poisson bracket. Therefore we

provide a connection between the classical and the quantum system in the classical limit

$$\lim_{\hbar\to 0}\frac{1}{i\hbar}[f,g]_* = \{f,g\}\,. \tag{2.80}$$

Mathematically it means that the new structure defined by the star product is anchored by the Poisson structure on the manifold.

3. Another requirement is that the product is associative which is a natural property if we want to have sensible products of more than two observables.

An abstract star product is a deformation of the classical product and the quantum algebra is a deformation of the classical one too. It can formally be written as

$$f * g = \sum_{n=0}^{\infty}(i\hbar)^n\mathcal{D}_n(f,g) = fg + i\hbar\mathcal{D}_1(f,g) + \mathcal{O}(\hbar^2)\,. \tag{2.81}$$

A noncommutative product in the algebra of functions on a Poisson manifold will then be called a star product if

$$\begin{aligned}
&1.\ \mathcal{D}_0(f,g) = fg\,, \\
&2.\ \mathcal{D}_1(f,g) - \mathcal{D}_1(g,f) = \{f,g\}\,, \\
&3.\ \sum_{i+j=n}\mathcal{D}_i(\mathcal{D}_j(f,g),h) = \sum_{i+j=n}\mathcal{D}_i(f,\mathcal{D}_j(g,h))\,.
\end{aligned} \tag{2.82}$$

In many cases we use a Hermitian star product, i.e. a star product that satisfies $\overline{f*g} = \bar{g}*\bar{f}$. Recall that the Moyal star product is a Hermitian product. While Hermitian products are almost exclusively considered in physics, non-Hermitian products can be very useful as we will discuss in relation to dissipation.

In the mathematical literature the existence of $*$-products on manifolds with Poisson structure has been proven by Kontsevich [53]. On a flat phase space all the possible star products are equivalent in the sense that for two different star products an

invertible *transition operator* T exists that relates them via

$$f *' g = T^{-1}(Tf * Tg)\,. \tag{2.83}$$

The equivalence is called *c-equivalence*, where "*c*" stands for Chevalley cohomology [2].

Two star products used in physics, other than the Moyal star product, are the standard star product:

$$f *_S g = f e^{i\hbar \overleftarrow{\partial}_q \vec{\partial}_p} g, \quad T = e^{-\frac{i\hbar}{2}\partial_q \partial_p} \tag{2.84}$$

and the normal star product:

$$f *_N g = f e^{i\hbar \overleftarrow{\partial}_a \vec{\partial}_{\bar{a}}} g, \quad T = e^{-\frac{\hbar}{2}\partial_a \partial_{\bar{a}}}\,, \tag{2.85}$$

where the functions a and $\bar{a}$ are the holomorphic variables which correspond to the creation and annihilation operators. One can also invert the direction of the action of the derivatives to get antistandard and antinormal $*$-products. According to [45], in $\mathbb{R}^{2n}$ $*$-products can be parametrized as:

$$f * g = f \exp[2\nu\, \overleftarrow{\partial}_a \vec{\partial}_a + 2\lambda\, \overleftarrow{\partial}_{\bar{a}} \vec{\partial}_{\bar{a}} + (\mu + \hbar/2)\, \overleftarrow{\partial}_a \vec{\partial}_{\bar{a}} + (\mu - \hbar/2)\, \overleftarrow{\partial}_{\bar{a}} \vec{\partial}_a] g\,. \tag{2.86}$$

The transition operator that defines the equivalence and will take us from the Moyal product to this one is

$$T = \exp[\mu \partial_a \partial_{\bar{a}} + \nu \partial_a^2 + \lambda \partial_{\bar{a}}^2]\,. \tag{2.87}$$

Recall that the Wigner-Weyl correspondence dictates the form of the Moyal $*$-product. Different orderings give rise to different star products and different Weyl maps. In

general we can write the Weyl map in the form [46]

$$\mathcal{W}_\lambda^{-1}(f) = \frac{1}{4\pi^2}\int d\,\xi\, d\eta\, dq\, dp f(q,p) e^{-i(\hat{q}-q)-i(\hat{p}-p)} e^{\lambda(\xi,\eta)}\,. \tag{2.88}$$

The argument of the extra exponential factor $e^{\lambda(\xi,\eta)}$ is a quadratic form of the integration variables

$$\lambda(\xi,\eta) = \frac{\hbar}{4}(\alpha\eta^2 + \beta\xi^2 + 2i\gamma\xi\eta)\,. \tag{2.89}$$

For different values of the parameter we recover the case of Weyl ordering (2.14)

$$qp \to \frac{1}{2}(\hat{q}\hat{p} + \hat{p}\hat{q}), \quad \alpha = \beta = \gamma = 0\,, \tag{2.90}$$

standard ordering

$$qp \to \hat{q}\hat{p}, \quad \alpha = \beta = 0, \gamma = 1\,, \tag{2.91}$$

and *antistandard ordering*

$$qp \to \hat{p}\hat{q}, \quad \alpha = \beta = 0, \gamma = -1\,. \tag{2.92}$$

When we work with holomorphic coordinates the same formula will give us the *normal ordering*

$$a\bar{a} \to \hat{a}\hat{a}^\dagger, \quad \alpha = 1, \beta = -1, \gamma = 0\,, \tag{2.93}$$

and the *antinormal ordering*

$$a\bar{a} \to \hat{a}^\dagger\hat{a}, \quad \alpha = -1, \beta = 1, \gamma = 0\,. \tag{2.94}$$

However one can write $*$-products which are not directly associated with an operator ordering and yet can be useful for physical application. For example the Husimi

$*$-product discussed in [71] is given by:

$$f *_H g = f * e^{\frac{\hbar}{2}(s^2 \overleftarrow{\partial}_q \vec{\partial}_q + s^{-2} \overleftarrow{\partial}_p \vec{\partial}_p)} g, \quad T = e^{\frac{\hbar}{4}(s^2 \partial_q^2 + s^{-2} \partial_p^2)} ., \tag{2.95}$$

Physically, it introduces coarse graining of the phase space. This is easily seen if we write the Husimi distribution as

$$\rho_H(q,p;t) = \frac{1}{\pi\hbar} \int dp' dq' \, \rho(q,p;t) \, e^{-(q-q')^2 - (p-p')^2} \, , \tag{2.96}$$

explicitly showing a Gaussian smoothing of the features of the Wigner function.

Another example is the Dito-Turrubiates $*$-product which introduces dissipation that we will study in the fourth chapter. The $*$-product in question can be viewed as a deformation of the Moyal $*$-product in terms of the dissipation parameter and as far as we know cannot be related to a sensible operator ordering.

The *c-equivalence* (cohomological equivalence) introduced by the transition operator T is, therefore, not necessarily a physical equivalence. It is purely mathematical and the particular star product used must be chosen by physical consideration.

Let us point out that the different distributions can be related to each other directly. A list of formulae can be found in [56].

2.7 The dynamical equations for deformation quantization

In deformation quantization the Schrödinger equation for the wave functions are replaced by the Moyal equation for the Wigner function. In order to describe a system in the framework of deformation quantization one should solve the Moyal equations and not use the Wigner-Weyl transform, except to compare. The equations of motion in deformation quantization are more complicated than the Schrödinger equation but

due to the $*$-product one can develop techniques similar to their operator counterparts. The Moyal equation has the form

$$i\hbar\frac{\partial\rho}{\partial t} + [\rho, H]_* \stackrel{\text{def}}{=} i\hbar\mathcal{L}\rho = 0\,. \tag{2.97}$$

As the equation of motion is first order in time any physically acceptable initial condition will determine the evolution of the system. For Hamiltonians that depend on the coordinates and the momenta only, the superoperator $i\hbar\mathcal{L}$ is also independent of time. Therefore if we have the Wigner function of the system at time $t = 0$ it evolves according to the formula:

$$\rho(q, p, t) = \exp\{t\mathcal{L}\}\rho(q, p, 0)\,. \tag{2.98}$$

This expression is trivially obtained from (2.97) and is only a formal solution.

Let us find an explicit formula for $\rho(t)$. The form of (2.97) demands that we write the Wigner function in a factorized form just as in the operator formalism:

$$\rho(q, p, t) = U(q, p, t) * \rho(q, p, 0) * \overline{U(q, p, t)}\,, \tag{2.99}$$

with $\bar{U}$ the complex conjugate[7]. Plugging (2.99) in (2.97) we get an equation for the factorizing function U

$$i\hbar\,\partial_t U(t) = H * U(t)\,. \tag{2.100}$$

We can solve this equation easily if we introduce a star exponential:

$$\mathrm{Exp}[*](x) \equiv \mathrm{Exp}_*(x) \stackrel{\text{def}}{=} \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n x^{*n}\,, \tag{2.101}$$

[7]In fact here we can substitute $\bar{U}$ with $U(-t)$ then we are dealing with dissipative systems since we no longer have unitary evolution.

where we have used the notation $x^{*n} = \underbrace{x * ... * x}_{n \text{ times}}$. Formal integration will give us the *time evolution function* for a time independent Hamiltonian:

$$U(q,p,t) = \mathrm{Exp}_*(tH) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-it}{\hbar}\right)^n H^{*n} \,. \tag{2.102}$$

The *star exponential* determines the evolution of the system and has the Hamiltonian as generator. That agrees with the operator formulation, since the $*$-exponential of the Hamiltonian is the symbol of the propagator. The unitary property of the time evolution function is expressed by a simple complex conjugation:

$$\overline{U(q,p,t)} * U(q,p,t) = U(q,p,t) * \overline{U(q,p,t)} = 1 \,, \tag{2.103}$$

along with $\overline{U(q,p,t)} = U(q,p,-t)$. Let us point out that the equation (2.100) has the form of the Schrödinger equation, however it cannot be found directly via Wigner-Weyl transform due to the presence of the wave function versus the density operator.

When the $*$-exponential converges to a distribution on the phase space, we can rewrite the solution in terms of *Fourier-Dirichlet series* ([2], [3]), where λ is a parameter taking values in some complex sequence that depends on the system:

$$\mathrm{Exp}_*(tf) = \sum_{\lambda \in \Lambda} \pi_\lambda(q,p) e^{-i\lambda t/\hbar} \,. \tag{2.104}$$

The $\pi_\lambda(q,p)$'s are just differentiable complex functions on the phase space and they are called *projectors*. Just like in Schrödinger quantum mechanics, a spectrum Λ of f can be defined and the values that λ take are the eigenvalues of f. In other words, a version of the spectral theory is emerging, one that does not require operators. For the Hamiltonian we have the following version

$$\mathrm{Exp}_*(tH) = \sum_{E} \rho_E(q,p) e^{-iEt/\hbar} \,. \tag{2.105}$$

Plugging that into the equation of motion (2.100) we get:

$$\sum_E \rho_E(q,p) E e^{-iEt/\hbar} = \sum_E H * \rho_E(q,p) e^{-iEt/\hbar} \,. \tag{2.106}$$

Taking into account that the exponentials are independent we get that in deformation quantization we can find stationary states solving

$$H * \rho_E(q,p) = E \ \rho_E(q,p) \,. \tag{2.107}$$

Now applying the same idea but to the equation of motion for the conjugate $\overline{U(t)}$:

$$\rho_{E'}(q,p) * H = E' \, \rho_{E'}(q,p) \,. \tag{2.108}$$

The hermiticity of the star and the reality if the energies allows us to identify ρ' and $\bar{\rho}$ for the same energies E which can also be found using that the evolution function is unitary. Any possible star-eigen ($*$-eigen) states will be idempotent and in particular orthogonal. To see this Let us have the diagonal Wigner functions for a given Hamiltonian H. Consider the expression $\rho_E * H * \rho_{E'}$

$$(\rho_E * H) * \rho_{E'} = E \rho_E * \rho_{E'} \,, \quad \rho_E * (H * \rho_{E'}) = E' \rho_E * \rho_{E'} \,, \tag{2.109}$$

By the virtue of associativity however those two expressions are the same so $(E - E')\rho_E * \rho_{E'} = 0$ which is an orthogonality condition for non-degenerate states. In other words if $E \neq E'$ then $\rho_E * \rho_{E'} = 0$, the compact form being

$$(\rho_E * \rho_{E'})(q,p) = \delta_{EE'} \rho_E(q,p) \,. \tag{2.110}$$

Therefore we can expand the Hamiltonian in terms of the stationary states:

$$H(q,p) = \sum_E E\rho_E(q,p)\,, \tag{2.111}$$

which trivializes the $*$-eigenvalue equations. Now, finally, we can write the complete solution in terms of the stationary Wigner functions using (2.99)

$$\begin{aligned}\rho(q,p,t) &= \sum_{EE'} e^{-it(E-E')/\hbar}\rho_E(q,p) * \rho(q,p,0) * \rho'_E(q,p) \\ &\stackrel{\text{def}}{=} \sum_{EE'} C_{EE'}\rho_{EE'}(q,p)e^{-it(E-E')/\hbar}\,.\end{aligned}$$

It is fairly obvious that we can use the Wigner transform on the Schrödinger equation and its generalization for density matrix. The functions $\rho_{EE'}$ correspond to the Wigner transform of $|E\rangle\langle E'|$, i.e. the non-diagonal matrix elements of the density operator. The *non-diagonal Wigner functions* $\rho_{EE'}$ satisfy

$$\begin{aligned}(H * \rho_{EE'})(q,p) &= E\,\rho_{EE'}\,, \\ (\rho_{EE'} * H)(q,p) &= E'\,\rho_{EE'}\,,\end{aligned} \tag{2.112}$$

with the relation $\rho_E = \rho_{EE}$ now becoming clear. They also satisfy orthogonality conditions [26]

$$\rho_{E_1E'_1} * \rho_{E_2E'_2} = \hbar^{-1}\delta_{E_1E'_2}\rho_{E_2E'_1}\,. \tag{2.113}$$

Let us point out that this presentation lacks mathematical rigor. However the intention is to show that a physicists with the mathematics of the 20th century could have easily worked their way through the quantum theory without a reference to Schrödinger equation whatsoever.

Integral form of the dynamical equations

When dealing with quantum mechanical systems, very often we get a Hamiltonian of the form $\hat{H} = p^2/2m + V(q)$. The explicit form of equation (2.97) is

$$i\hbar\frac{\partial\rho}{\partial t} = -\frac{i\hbar p}{m}\,\frac{\partial\rho}{\partial q} + \sum_{n=0}^{\infty}\frac{2}{(2n+1)!}\left(\frac{i\hbar}{2}\right)^{2n+1}\frac{\partial^{2n+1}V}{\partial q^{2n+1}}\,\frac{\partial^{2n+1}\rho}{\partial p^{2n+1}}\,. \tag{2.114}$$

The form suggests it is valid if all the derivatives of the potential exist. However we will encounter various walls and barriers, which are discontinuous. This problem creates a curious phenomenon. The Wigner functions found via the Wigner-Weyl correspondence and the Wigner functions found by solving the $*$-eigenvalue equations with the bulk Hamiltonian are different. This is because the non-linearity of the equations produces highly nontrivial effects on the boundary. Mathematically, the derivatives of the sharp potentials may exist as distributions. Due to the pseudo-differential nature of the $*$-product, it may have infinite number of non-zero derivative terms. Solving the equations piece-wise will ignore those boundary terms. This will change drastically the way matching is done in deformation quantization as we will see in the next chapter.

However deformation quantization is well equipped to tackle this problem. If we insist on differential forms of the dynamical equations we can proceed to the next chapter where some of the issues are discussed and resolved. On the other hand, recall that an integral form of the star product exists and it does not require the functions to be differentiable, instead it only requires them to be integrable. Using the integral representation (2.39) of the $*$-product we can write (2.97) as

$$\frac{\partial\rho}{\partial t} = -\frac{p}{m}\,\frac{\partial\rho}{\partial q} + \int_{-\infty}^{+\infty} d\eta\,\rho(q,p+\eta)K(q,\eta) \tag{2.115}$$

with a kernel we can calculate from the potential:

$$K(q,\eta) = \frac{i}{\pi^2\hbar^2}\int_{-\infty}^{+\infty} d\zeta[V(q+\zeta) - V(q-\zeta)]e^{-\frac{2i}{\hbar}\eta\,\zeta}\,. \tag{2.116}$$

This form of the dynamical equation may be more difficult to solve but it has a more general form[8] that includes all integrable potentials of physical interest [56], e.g. step potentials, finite wells, delta function, etc.[9]

Schrödinger equation as underlying structure for the Moyal star product

The Wigner-Weyl transform can relate deformation quantization results to standard operator quantization results. Moreover if deformation quantization is taken as the primary quantization technique one can still derive the Schrödinger equation within the phase space quantum mechanics framework. Let us see how the Schrödinger equation emerges as an underlying structure of the Moyal equation

Suppose we have any coordinate and time-independent potential as it is customary in quantum mechanics - $H(q,p) = \frac{p^2}{2m} + V(q)$. The $*$-eigenvalue equations will then be:

$$H*\rho = E\rho \Leftrightarrow \left(\frac{p^2}{2m} - E\right)\rho - \frac{\hbar^2}{8m}\partial^2_{qq}\rho - \frac{i\hbar p}{2m}\partial_q\rho + \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\hbar}{2}\right)^n \partial_q^n V \partial_p^n \rho = 0\,, \tag{2.117}$$

$$\rho * H = E'\rho \Leftrightarrow \left(\frac{p^2}{2m} - E'\right)\rho - \frac{\hbar^2}{8m}\partial^2_{qq}\rho + \frac{i\hbar p}{2m}\partial_q\rho + \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\left(\frac{i\hbar}{2}\right)^n \partial_q^n V \partial_p^n \rho = 0\,. \tag{2.118}$$

Solving the equations in this form can be very challenging. However there is an

[8] Recall that an integral form of the $*$-product exists for integrable functions and therefore it is more general. Only in the case when the functions are smooth the integral and pseudodifferential forms are equivalent [56].

[9] Note that this equation cannot treat infinite wall for example, since it is not integrable. However it is physically important. The solution of this problem and related topics will be discussed this in detail in the next chapter. However, the short answer is that we need to modify the equations or the Hamiltonian. Alternatively we can recover the infinite wall as a limit of smooth potentials.

apparent asymmetry between q and p that suggests the use of Fourier transform for p only.

$$-\frac{1}{4}\partial^2_{qq}f(q,\xi) - \partial^2_{q\xi}f(q,\xi) - \partial^2_{\xi\xi}f(q,\xi) + [V(q+\xi/2) - E]f(q,\xi) = 0\,, \tag{2.119}$$

$$-\frac{1}{4}\partial^2_{qq}f(q,\xi) + \partial^2_{q\xi}f(q,\xi) - \partial^2_{\xi\xi}f(q,\xi) + [V(q-\xi/2) - E']f(q,\xi) = 0\,, \tag{2.120}$$

where $\mathcal{F}_\xi(\rho(q,p)) = f(q,\xi)$ is the Fourier transform of the Wigner function. The PDE' s can be written in their canonical form using the following transformations: $u = q - \xi/2$, $v = q + \xi/2$:

$$\partial^2_{uu}f(u,v) + [E - V(u)]f(u,v) = 0\,, \tag{2.121}$$

$$\partial^2_{vv}f(u,v) + [E' - V(v)]f(u,v) = 0\,. \tag{2.122}$$

We recover the Schrödinger equation. So, in a sense, even if we first discovered deformation quantization, we would have to deal with the Schrödinger equation instead of the $*$-eigenvalue equations for simplicity. This is something we have already seen in the case of Korteweg-de Vries equation and seems to be the case for other nonlinear integrable systems.

It is interesting to notice that when we deal with supersymmetric quantum mechanics the Schrödinger equation appears again (see Appendix A). The method we use in dealing with factorisable Hamiltonians is called the Darboux construction and in some form has been around since the 19th century. The point is that even if deformation quantization happened to be the first approach to have been discovered the Schrödinger equation would still play a central role even if just for technical reasons. Also a direct integration over the coordinates or the momentum can give us the regular interpretation of the wave function. From this argument is not clear whether or not operators follow naturally from deformation quantization. So far we have shown

that they are not needed so the most likely answer is "no". However a scenario like the above has one very attractive feature. Its postulates are straightforward generalizations of classical physics and the wave functions and their probabilistic interpretation are derived from those. This will also allow the physical boundary conditions to be imposed on the wave function that we know from textbook quantum mechanics.

2.8 Simple harmonic oscillator

The simple harmonic oscillator is a perfect example to illustrate those techniques because it is not too complicated and yet non-trivial. For simplicity we set $m = \omega = 1$. Therefore the system will have Hamiltonian given by $H = (p^2 + q^2)/2$.

Analytic method

The simple quadratic form of the Hamiltonian suggests that using Bopp shifts (2.32) is the easiest way to write the $*$-product of the Hamiltonian and the Wigner function:

$$\left[\frac{1}{2}\left(p + \frac{i\hbar}{2}\partial_q\right)^2 + \frac{1}{2}\left(q + \frac{i\hbar}{2}\partial_p\right)^2\right]\rho = E\rho. \tag{2.123}$$

Explicitly we can write the above equation as a a polynomial in $\hbar$ thus recovering the same result as if we used (2.31):

$$\frac{1}{2}(q^2 + p^2)\rho + \frac{i\hbar}{2}(q\partial_p\rho - p\partial_q\rho) - \frac{\hbar^2}{8}(\partial_{qq}^2 + \partial_{pp}^2)\rho = E\rho. \tag{2.124}$$

For the harmonic oscillator the equation is relatively simple due to the fact that the Hamiltonian is a quadratic polynomial in q and p. The infinite series of derivatives in the expression for the star product terminates after the third term.

To solve (2.124) note that the diagonal eigenstates are Wigner function is real for pure states. Therefore, we can separate the real from the imaginary part of the

equation. Since the Wigner function does not have an imaginary part the equations decouple:

$$(q\partial_p - p\partial_q)\,\rho = 0\,, \tag{2.125}$$

$$[\,q^2 + p^2 - \frac{1}{4}(\partial_q^2 + \partial_p^2) - 2E\,]\,\rho = 0\,. \tag{2.126}$$

The first equation can be solved using the characteristics method. Along the characteristics partial differential equations become ordinary. In this case $q^2 + p^2 = C$, where C is a constant, gives a one-parameter family of curves and the variable we use to parametrize a characteristic turns out to be the Hamiltonian. Therefore $\rho(q,p) = \rho((q^2+p^2)/2) = \rho(H)$. Using the substitution $z = 4H/\hbar$ we transform equation (2.126) into an ordinary differential equation

$$(z/4 - \partial_z - z\partial_{zz}^2 - E/\hbar)\rho = 0\,. \tag{2.127}$$

This equation can be explored for asymptotic solutions in order to suggest what form the will solutions have. At $z \to \infty$ we find that the equation and solutions are:

$$\partial_{zz}^2\rho - \frac{\rho}{4} = 0,\ \rho(z) = C_1 e^{z/2} + C_2 e^{-z/2}\,. \tag{2.128}$$

For normalizable Wigner function we must discard the unbounded solution, i.e. put $C_1 = 0$. Now we can factorize $\rho(z)$ into an exponential part and a part that we need to determine from the original differential equation. This equation can be transformed using the substitution $\rho(z) = \exp(-z/2)f(z)$ into a known ordinary differential equation

$$\left[\, z\partial_{zz}^2 + (1-z)\partial_z + E/\hbar - 1/2 \,\right] f(z) = 0\,, \tag{2.129}$$

which has two independent solutions - the Laguerre functions and the Tricomi con-

fluent hypergeometric function:

$$f(z) = C_1 L_{E/\hbar - 1/2}(z) + C_2 U(-E/\hbar + 1/2, 1, z)\,. \tag{2.130}$$

However only for integer values of $E/\hbar - 1/2$ we have normalizable solutions - the Laguerre polynomials:

$$L_n(z) = \frac{e^z}{n!}\frac{\partial^n(e^{-z}z^n)}{\partial z^n}\,. \tag{2.131}$$

They are relatively easy to find for small n

$$L_0 = 1,\, L_1(z) = 1 - z,\, L_2(z) = 1 - 2z + z^2/2\,, \tag{2.132}$$

$$L_3(z) = 1 - 3z + (3z^2)/2 - z^3/6\,,\, ... \tag{2.133}$$

A pattern is already emerging for the explicit formula for every $n \in \mathbb{N}$:

$$L_n(z) = \sum_{k=0}^{n} \frac{(-1)^k}{k!}\binom{n}{n-k} z^k\,. \tag{2.134}$$

The final solution for the states and the corresponding energies can be written as

$$\rho_n(z) = \frac{(-1)^n}{\pi\hbar} e^{-2H/\hbar} L_n(4H/\hbar),\;\; E_n = (n + 1/2)\hbar,\;\; n \in \mathbb{N}\,. \tag{2.135}$$

The significance of this calculation is in the fact that we did not at any point use operators or wave functions. From the classical Hamiltonian following deformation quantization techniques only we derived the spectrum for the simple harmonic oscillator. Also using the quasi-probability distributions we just found we can calculate anything that we can in operator formalism.

Let us point out that for many simple potentials this program works well, while for others the equations of motion, will be too complicated to be approached like this. For example even for simple harmonic oscillator we encounter difficulties when

we try to apply the outlined method in the case of non-diagonal eigenfunctions. The off-diagonal Wigner functions have imaginary parts which we have to take into account. That leads to a system of two equations for the real and imaginary part that are coupled and complicated. Clearly different methods will be effective in different situations.

Algebraic method

We will now present a re-formulation of the algebraic method from operator quantum mechanics. This alternative method based on the factorization of the Hamiltonian. The transition to phase space quantum mechanics is almost trivial so we will not include much detail. However it is useful toy model to study since its basic idea of factorization can be extended for so-called supersymmetric potentials (see [79]). For an example, please see Appendix A, where the non-trivial problem of deformation quantization for Morse potential is treated.

We first define the holomorphic variables in order to factorize the Hamiltonian, i.e. to write it as a $*$-product of two functions. For simplicity we take $m = \omega = 1$:

$$a = \frac{1}{\sqrt{2\hbar}}(q + ip)\,, \qquad \bar{a} = \frac{1}{\sqrt{2\hbar}}(q - ip)\,. \tag{2.136}$$

Clearly those variables are the counterparts of the creation and annihilation operators. They satisfy commutation relations identical to the operator versions, except that the operator product is replaced by the $*$-product

$$[a, \bar{a}]_* = a * \bar{a} - \bar{a} * a = 1\,. \tag{2.137}$$

The Hamiltonian can now be be represented as a factor of those two using the $*$-

product and its form is identical to operator counterpart

$$H = \hbar(\bar{a} * a + 1/2)\,. \tag{2.138}$$

What follows is essentially a repetition of the standard textbook argument so we omit it. However note that now we can explicitly compute the ground state Wigner function

$$a * \rho_0 = \rho_0 * \bar{a} = 0\,. \tag{2.139}$$

The equations can be written explicitly using the Bopp shifts as before. Solving those simultaneously

$$x\rho + \frac{\hbar}{2}\frac{\partial \rho}{\partial q} = 0, \quad p\rho + \frac{\hbar}{2}\frac{\partial \rho}{\partial p} = 0\,, \tag{2.140}$$

will, of course reproduce the ground state from before $\rho \propto e^{-(q^2+p^2)/\hbar}$. From this expression every excited state can be calculated by differentiating the ground state certain amount of times:

$$\rho_{mn} \propto \bar{a}^m * \rho_0 * a^n\,. \tag{2.141}$$

The star exponential method

This example will illustrate how in certain cases is easy enough to determine all the states just form the spectral decomposition of the evolution function. We start with the equation (2.100) and solve directly for the star exponential. The explicit form is

$$4i\hbar\partial_t Exp_*(tH) = \left[4H - \hbar^2\omega^2\partial_H - \hbar^2\omega^2 H\partial_H^2\right] Exp_*(tH)\,. \tag{2.142}$$

We then get the solution:

$$Exp_*(tH) = \frac{e^{\frac{2H}{i\hbar\omega}\tan\frac{\omega t}{2}}}{\cos(\omega t/2)}\,. \tag{2.143}$$

To find the Fourier-Dirichlet expansion we use the fact that the exponential above is in the form of a generating function:

$$\frac{1}{1+s}\exp\left(\frac{zs}{1+s}\right)=\sum_{n=0}^{\infty}(-s)^n L_n(z)\,. \tag{2.144}$$

which then gives the stationary states as projectors after we compare the corresponding terms

$$\rho_n(q,p)=2(-1)^n e^{-2H/\hbar\omega}L_n\left(4H/\hbar\omega\right)\,. \tag{2.145}$$

Clearly, the simple harmonic oscillator is simple enough to be treated in any of those approaches. That is what makes it a perfect example to illustrate some of the techniques one can use in deformation quantization. In general, a direct application of any of those might be difficult – an example of a system that cannot be treated as above is the Morse potential, discussed in the next chapter. Finding general solutions in pure deformation quantization fashion is a challenging problem.

2.9 Fermionic star products

So far we have been concerned with building the deformation quantization method consistently, without reference to operator mechanics, except to show correspondences. We also pointed out what the relationships are. There is an obvious omission, however. To be an independent quantum formulation deformation quantization must include the treatment of spin. There are two methods that reproduce spin.

2.9.1 The Stratonovich-Weyl quantization technique

Here we will present a spin-$\frac{1}{2}$ particle as treated in deformation quantization, using a method first introduced by Stratonovich. Simply put, we choose a two dimensional sphere as the phase space, define a Wigner-Weyl map from physical considerations

and then write the $*$-product that corresponds to that map.

To understand why this program makes sense let us recall some basic facts in relation to coadjoint orbits. Recall that a Lie group G defines an *inner automorphism*

$$A(g) : h \to ghg^{-1}, \quad g, h \in G\,. \tag{2.146}$$

Consider a differentiable map between manifolds $f : M \to N$. The *differential (tangent) map* at point p is an induced map $f_{*p} : T_pM \to T_{f(p)}N$ defined via

$$(f_{*p}v)(g) = v(g \circ f)\,, \quad v \in T_pM\,, \tag{2.147}$$

where $g \in \mathcal{F}(N)$ is any test smooth function. In other words the tangent map acting on a vector v its just the directional derivative with respect to v.

In the Lie algebra $\mathfrak{g}$ of G that defines the map $Ad(g) \stackrel{\text{def}}{=} A_{*e}(g) : \mathfrak{g} \to \mathfrak{g}$. The *adjoint representation* is the map $g \mapsto Ad(g)$. It is a homomorphism between G and $\mathrm{Aut}(\mathfrak{g})$ and also a differentiable map. All abstract Lie groups are locally isomorphic to matrix groups. In terms of matrices we can write it as

$$Ad(g)X = gXg^{-1}\,, \quad g \in G \text{ and } X \in \mathfrak{g}\,. \tag{2.148}$$

Let us now consider a representation π of the group G in a linear space V. The *dual representation* (π^*, V^*) is defined as follows

$$\pi^*(g) \stackrel{\text{def}}{=} \pi(g^{-1})^*, \tag{2.149}$$

where the asterisk indicates dual: V^* is the dual space to V and the dual operator is defined via

$$\langle \pi^* f, v\rangle = \langle f, \pi v\rangle, \quad v \in V, f \in V^*\,. \tag{2.150}$$

For deformation quantization the representation of interest is the *coadjoint representation* K of G in $\mathfrak{g}^*$ which is simply the dual of the adjoint one, i.e $K(g) \stackrel{\text{def}}{=} Ad^*(g) = Ad(g^{-1})$. The orbits of G in $\mathfrak{g}^*$ are called *coadjoint orbits*. The orbit method was developed by Kirillov and the most complete and comprehensive work on the subject is his book [51]. Coadjoint orbits are even-dimensional manifolds with a "natural way" of defining a symplectic structure ω, i.e. they are symplectic manifolds. "Natural way" means that we do not need to introduce a new structure on the coadjoint orbit Ω:

$$\omega_{\Omega,F}(K_*(X)F, K_*(Y)F) = \langle F, [X,Y]\rangle, \qquad X, Y \in \mathfrak{g}, F \in \mathfrak{g}^*\,, \tag{2.151}$$

where K_* is the infinitesimal version of the coadjoint representation, i.e. the one of $\mathfrak{g}$ in $\mathfrak{g}^*$. The symplectic form defined with this equation is also G-invariant.[10] For all our purposes phase spaces are symplectic manifolds[11] and therefore the coadjoint orbits can be thought as phase spaces.

Let us recall that in standard operator quantum mechanics j-spin, $j \in \{\frac{1}{2}, 1, \frac{3}{2}, ...\}$, can be represented by operators

$$J^2|jm\rangle = j(j+1)|jm\rangle, \qquad J_z|jm\rangle = m|jm\rangle, \qquad (\hbar = 1) \tag{2.152}$$

acting on $2j+1$ dimensional complex linear spaces $\mathbb{C}^{2j+1}$. The eigenstates $|jm\rangle$ form an orthonormal basis. Each linear space $\mathbb{C}^{2j+1}$ carries a representation π_j of the Lie group $SU(2)$. The coadjoint orbits of $SU(2)$ are simply spheres with different radii. The symplectic form on a sphere is given locally by the 2-form

$$\omega(\vec{n}) = d\phi \wedge \sin\theta\, d\theta, \qquad \vec{n} \stackrel{\text{def}}{=} (\theta, \phi) \tag{2.153}$$

[10] For details see Appendix B.

[11] Star products exist more generally on Poisson manifolds. as shown by Kontsevich [53].

in a fixed chart.

In classical mechanics $\mathbb{R}^{2n}$ is the phase space in the majority of the cases. When systems with constrains are involved we can have curved noncompact symplectic manifolds as phase spaces. However compact manifolds are considered unphysical. In quantum mechanics this is clearly not the case. If the symmetry group has compact coadjoint orbits then the relevant phase space will be compact. The emergence of S^2 follows from $G = SU(2)$, however we can generalize this technique for other groups of physical interest.

Let us recap - the most important feature of deformation quantization is that we do not work with operators. Instead we work with functions on the phase space. The Wigner transform gives us a way to switch from operator quantum mechanics to quantum mechanics on phase space. The properties of the Wigner transform that we studied in the spin zero case are not going to be changed much. The new "Wigner-Weyl" correspondence $\hat{f} \leftrightarrow \mathcal{W}(\hat{f}) \stackrel{\text{def}}{=} f(\theta, \phi) = f(\vec{n})$ must satisfy some physical and mathematical properties (see [69], [74] and [39]) in order to be a generalization of the bosonic Wigner-Weyl map.

1. *Linearity*: $\mathcal{W}(\lambda\hat{f}+\mu\hat{g}) = \lambda\mathcal{W}(\hat{f})+\mu\mathcal{W}(\hat{g})$. One may be tempted to drop the linearity property in attempt to obtain a more general map in deformation quantization of particles with non-zero spin. However, a non-linear Wigner-Weyl correspondence leads to inconsistencies and insurmountable difficulties with the probability interpretation.

2. *$\mathcal{W}$ is bijective map.* In other words for all operators $\hat{f}$ an image $\mathcal{W}(\hat{f})$ will exists in the algebra of the phase space functions. The opposite will also be true. This is essential since we want the quantum mechanics to be operator and wave function free as in the $\mathbb{R}^{2n}$ case. A crucial observation is that the Wigner- Weyl correspondence is a homomorphism and we would like to preserve that property in the case of the compact phase space S^2.

3. *Reality*: $\mathcal{W}(\hat{f}^\dagger) = \overline{\mathcal{W}(\hat{f})}$. The reality of the Wigner function needs to be guaranteed. Since we do not have the explicit form of the Stratonovich-Weyl correspondence we need to impose that as a condition. In other words the symbol of an operator can be real if and only if the operator is Hermitian.

4. *Traciality*. Physically, we expect to recover the same average for a physical observable using operator quantum mechanics and phase space averaging in deformation quantization, using the density operator. More generally:

$$\mathrm{Tr}(\hat{f}\hat{g}) = \frac{2j+1}{4\pi}\int_{S^2} d\vec{n}\,\mathcal{W}(\hat{f})\mathcal{W}(\hat{g}) = \frac{2j+1}{4\pi}\int_{S^2} d\vec{n} f(\vec{n})g(\vec{n}), \tag{2.154}$$

where the normalization constant is put in for later convenience. Unlike the $\mathbb{R}^{2n}$ case where the boundary terms disappear so we have (2.61), in the S^2 case we need to construct the $*$-product this way.

5. *Standardization*.

$$\mathrm{Tr}(\hat{f}) = \frac{2j+1}{4\pi}\int_{S^2} d\vec{n}\,\mathcal{W}(\hat{f})\,. \tag{2.155}$$

This can be easily obtained from (4.) in the finite-dimensional space. However, in general we need to add this condition in order to relate the identity operator to unity as we are used to.

6. *Covariance*. This property will reflect the spherical symmetry of the system:

$$\mathcal{W}(g\cdot\hat{f}) = g\cdot\mathcal{W}(\hat{f})\,, \tag{2.156}$$

relating the transformation properties of the operator algebra

$$g\cdot\hat{f} = \pi_j(g)\,\hat{f}\,\pi_j^{-1}(g) \tag{2.157}$$

to those of the functional algebra on the sphere

$$g \cdot f(\vec{n}) = f(g^{-1} \cdot \vec{n})\,. \tag{2.158}$$

We used here a particular representation of $SU(2)$ — $\pi_j(g)$ and we rewrote the transformation of a scalar function in a form similar to the operator transformation.

We will use the term *Stratonovich-Weyl correspondence* to replace Wigner-Weyl correspondence in the spin case. Also we define the *Stratonovich-Weyl symbol* of $\hat{f}$ to be $f \stackrel{\text{def}}{=} \mathcal{W}(\hat{f})$ obeying the above properties.

Before we continue and show how the symbol can be found, let us give the explicit form for the Weyl map:

$$\begin{aligned} \hat{f} &= \sqrt{\frac{2j+1}{4\pi}} \int_{\mathbf{S}^2} f(\vec{\mathrm{n}}) \sum_{l=0}^{2j} \sum_{m=-l}^{l} \mathbf{C}^{j*}_{lm}\; Y_{lm}(\vec{\mathrm{n}})\; d\vec{\mathrm{n}} = \\ &= \sum_{l=0}^{2j} \sum_{m=-l}^{l} \mathbf{C}^{j*}_{lm} \sqrt{\frac{2j+1}{4\pi}} \int_0^{2\pi} \int_{-\pi}^{\pi} f(\theta,\phi) Y_{lm}(\theta,\phi) \sin\theta\; d\theta\; d\phi \end{aligned} \tag{2.159}$$

where $\mathbf{C}^{j*}_{lm}$ are given matrices, whose matrix elements (up to a sign) are the Clebsch-Gordan coefficients. The Wigner transform on S^2 is then expressed in trace form using the *Stratonovich-Weyl quantizer*:

$$f(\vec{n}) = \mathrm{Tr}\left(\hat{f} \sum_{l=0}^{2j} \sum_{m=-l}^{l} \mathbf{C}^{j*}_{lm}\; Y_{lm}(\vec{\mathrm{n}}) \right), \tag{2.160}$$

where $Y_{lm}(\theta,\phi)$ are the spherical harmonics.

Stratonovich-Weyl operator kernel

We will show how can we find the form of the Stratonovich-Weyl correspondence. Assume that for a particular representation of $SU(2)$ — $\pi_j(g)$ an operator $\hat{w}_j(\vec{n})$

exists such that

$$f \stackrel{\text{def}}{=} \mathcal{W}(\hat{f}) = \text{Tr}\left(\hat{f}\hat{w}_j(\vec{n})\right) , \tag{2.161}$$

in close analogy with the $\mathbb{R}^{2n}$ case. The operator valued map on the sphere $\hat{w}_j(\vec{n})$ is called *Stratonovich-Weyl operator kernel*. Now we can use the properties 1.– 6. we postulated earlier. Let us point out that we can write the operator knowing its symbol

$$\hat{f} = \frac{2j+1}{4\pi}\int_{S^2} d\vec{n}\, f(\vec{n})\hat{w}_j(\vec{n}), \tag{2.162}$$

using the same kernel. Now the problem of showing that the homomorphism between the operator algebra and the functional algebra with the properties the properties 1.– 6. translates into a problem for the kernel $\hat{w}_j(\vec{n})$.

Taking the conjugate of f and using the reality condition (3.) we determine that

$$i.\ \hat{w}_j^\dagger(\vec{n}) = \hat{w}_j(\vec{n}), \forall \vec{n} \in S^2 , \tag{2.163}$$

i.e. the kernel is a self-adjoint operator for all real symbols. Now we can substitute $\hat{\mathbf{1}}$ for $\hat{f}$ and we get

$$ii.\ \int_{S^2} \hat{w}_j(\vec{n})d\vec{n} = 4\pi\hat{\mathbf{1}}/(2j+1) . \tag{2.164}$$

The traciality condition can be incorporated if we use the representation of the operator (2.162) in (2.161):

$$f(\vec{n}) = \text{Tr}(\hat{f}\hat{w}_j(\vec{n})) = \frac{2j+1}{4\pi}\int_{S^2} d\vec{m}\, \text{Tr}[\hat{w}_j(\vec{n})\hat{w}_j(\vec{m})]f(\vec{m}) . \tag{2.165}$$

Now using (2.161) one more time:

$$\text{Tr}(\hat{f}\hat{w}_j(\vec{n})) = \frac{2j+1}{4\pi}\int_{S^2} d\vec{m}\, \text{Tr}[\hat{w}_j(\vec{n})\hat{w}_j(\vec{m})]\text{Tr}[\hat{w}_j(\vec{m})\hat{f}] . \tag{2.166}$$

Taking the trace acting on the $\hat{f}$ term out of the integral and eliminating it from both sides leads to

$$iii.\ \hat{w}_j(\vec{n}) = \frac{2j+1}{4\pi}\int_{S^2} d\vec{m}\,\mathrm{Tr}[\hat{w}_j(\vec{n})\hat{w}_j(\vec{m})]\hat{w}_j(\vec{m})\,. \tag{2.167}$$

The final property can be derived trivially by using (6.) and the definition of action of $SU(2)$ on the operator algebra. After switching from g to g^{-1} we get

$$iv.\ \hat{w}_j(g\cdot\vec{n}) = \pi_j(g)\hat{w}_j(\vec{n})\pi_j^{-1}(g)\,, \tag{2.168}$$

i.e. the transformation rule for the Stratonovich-Weyl operator kernel.

Existence of the Stratonovich-Weyl kernel

We need to implement those conditions in a way that will give us the explicit form of the kernel. To do that we will write it in an arbitrary basis and see what happens to the matrix elements when *i.* – *iv.* are imposed.

$$\hat{w}_j(\vec{n}) \stackrel{\mathrm{def}}{=} \sum_{i,k=-j}^{j} Z^j_{ik}(\vec{n})|ji\rangle\langle jk|\,. \tag{2.169}$$

Imposing $(iv.)$ relates the matrix elements of the kernel to those of the representation π_j via the formula

$$Z^j_{ik}(g\cdot\vec{n}) = \langle ji|\hat{w}_j(g\cdot\vec{n})|jk\rangle = \sum_{m,n=-j}^{j}\mathcal{D}^j_{im}\mathcal{D}^{j^*}_{kn}Z^j_{mn}(\vec{n})\,. \tag{2.170}$$

Now we can use that a product of two matrix elements $\mathcal{D}^j_{mn}(g) = \langle jm|\pi_j(g)|jn\rangle$ can be expressed as sum over $\mathcal{D}$'s using the Clebsch-Gordan coefficients:

$$\mathcal{D}^j_{im}\mathcal{D}^{j^*}_{kn} = \sum_{l=0}^{2j}\frac{2l+1}{2j+1}C^{j\ l\ j}_{i,k-i,k}C^{j\ l\ j}_{m,n-m,n}\mathcal{D}^{j^*}_{k-i,n-m}\,. \tag{2.171}$$

We can now rewrite (2.170) using the above formula and relabel the indices:

$$Z^j_{ik}(g\cdot\vec{n}) = \sum_{l=0}^{2j}\sum_{p,n}(-1)^{2j-i-m}C^{j\ j\ l}_{i,-k,i-k}C^{j\ j\ l}_{m,-m-n,-n}\mathcal{D}^{j^*}_{k-i,n}(g)Z^j_{m,n+m}(\vec{n})\,. \tag{2.172}$$

The point of this whole exercise is that mathematical quantities with the above transformation properties on the sphere are already known. To see that we define

$$\tilde{Y}_{lm}(g\cdot\vec{n}) \stackrel{\text{def}}{=} \sum_{n=-j}^{j}(-1)^{j-n}C^{j\ j\ l}_{n,-n-m,-m}Z^j_{n,m+n}(\vec{n})\,, \tag{2.173}$$

which using the orthogonality properties of the Clebsch-Gordan coefficients leads to the transformation rule obeyed by the spherical harmonics:

$$\tilde{Y}_{lm}(g\cdot\vec{n}) = \sum_{n=-j}^{j}\mathcal{D}^{j^*}_{mn}(g)\tilde{Y}_{ln}(\vec{n})\,. \tag{2.174}$$

If c^{lk}_{mn} are the matrix elements of the intertwiner of π_k and π_j by Schur's lemma we get $c^{lk}_{mn} = \lambda^j_l\delta_{lk}\delta_{mn}$ and therefore $\tilde{Y}_{lm} = \lambda^j_l Y_{lm}$ With that in mind we can write 2^{2j} different kernels. In [74] one can find that the constants can be further constrained to be:

$$\lambda^l_j = \varepsilon^l_j\sqrt{4\pi/(2j+1)},\quad \lambda^0_j = \sqrt{4\pi/(2j+1)},\quad \varepsilon^l_j = \pm 1\,. \tag{2.175}$$

Finally we chose $\varepsilon^l_j = 1$ to recover the known physics.

We can now invert (2.173) to find the expression for the matrix elements of the Stratonovich-Weyl operator kernel

$$Z^j_{rs}(\vec{n}) = (-1)^{j-r}\sum_{l=0}^{2j}\lambda^j_l C^{j\ j\ l}_{r,-s,r-s}Y_{l,s-r}(\vec{n})\,. \tag{2.176}$$

To further streamline the expression and eliminate the explicit basis dependence, we

use the Clebsch-Gordan coefficients to define the following matrices:

$$\langle jr|\mathbf{C}^{j^*}_{lm}|js\rangle = (-1)^{j-r} C^{j\ j\ l}_{r,-s,-m}\,. \tag{2.177}$$

Finally we arrive at the expression for the Stratonovich-Weyl operator kernel (quantizer)

$$\hat{w}_j(\vec{n}) = \sum_{l=0}^{2j}\sum_{m=-j}^{j}\sqrt{\frac{4\pi}{2j+1}}\mathbf{C}^{j^*}_{lm}Y_{lm}(\vec{n}). \tag{2.178}$$

and the equations (2.159) and (2.160).

Clearly the deformation quantization program can be applied here, since we have an analog of the Wigner-Weyl correspondence which allows us to work with functions on the sphere only, without reference to operators.

Stratonovich-Moyal star product

Let us now determine what $*$-product will emerge from the Stratonovich-Weyl correspondence. Recall that the Moyal product defines a homomorphism between the operator algebra and the algebra of phase space functions. We will exploit the homomorphism property to relate the product of operators to the product of two Stratonovich-Weyl symbols.

$$(\mathcal{W}(\hat{f}\hat{g}))(\vec{n}) = \mathrm{Tr}[\hat{w}_j(\vec{n})\hat{f}\hat{g}] \propto \int_{S^2} d\vec{m}\int_{S^2} d\vec{k}\,\mathrm{Tr}[\hat{w}_j(\vec{n})\hat{w}_j(\vec{m})\hat{w}_j(\vec{k})]f(\vec{m})g(\vec{k}) \tag{2.179}$$

after we have substituted (2.162) for the operators $\hat{f}$ and $\hat{g}$. From here we can derive the integral representation of the Moyal $*$-product counterpart. Let us first define the kernel using the matrix elements of the Stratonovich-Weyl operator kernel

$$K_j(\vec{k},\vec{m},\vec{n}) = \frac{(2j+1)^2}{16\pi^2}\sum_{r,s,t=-j}^{j} Z^j_{rs}(\vec{n})Z^j_{st}(\vec{m})Z^j_{tr}(\vec{k})\,. \tag{2.180}$$

With this we can write the Stratonovich-Moyal $*$-product in the familiar form:

$$(f * g)(\vec{n}) = \int_{S^2} d\vec{m} \int_{S^2} d\vec{k}\, K_j(\vec{k}, \vec{m}, \vec{n}) f(\vec{m}) g(\vec{k})\,. \tag{2.181}$$

Now it is relatively easy using the properties of the kernel to derive the tracial property of the $*$-product:

$$\int_{S^2} d\vec{n} (f * g)(\vec{n}) = \int_{S^2} d\vec{n} f(\vec{n}) g(\vec{n})\,, \tag{2.182}$$

as well as to show that it is covariant:

$$(f * h)(g \cdot \vec{n}) = f(g \cdot \vec{n}) * h(g \cdot \vec{n}), \quad \forall g \in SU(2). \tag{2.183}$$

Those two conditions are very important – as we discussed previously (2.182) reflects the cyclic property of the trace and (2.183) simply states that the $*$-product preserves the transformation property of functions. Another important property is rotational invariance:

$$K_j(g \cdot \vec{k}, g \cdot \vec{m}, g \cdot \vec{n}) = K_j(\vec{k}, \vec{m}, \vec{n})\,. \tag{2.184}$$

This property constrains the form of the kernel and provides alternative method to find it (see [74] for $j = 1/2$ example).

A differential form of the $*$-product can be derived from the integral representation. The full derivation can be found in [52]; here we only outline the ideas behind it. Let us assume as usual that the $*$-product can be written as a bi-differential operator

$$f * g = \hat{\mathcal{D}}_j(f, g)\,. \tag{2.185}$$

Any two operators $\hat{f}$ and $\hat{g}$ can be expanded in terms of $\mathbf{C}^{j*}_{lm}$ since the latter form a basis. Then the idea is to express a product $\hat{f}\hat{g}$ in terms of the basis and express it via the corresponding Stratonovich-Weyl operator kernel. Comparing with the equation

(2.185) above one can write the bi-differential operator in the form

$$\hat{\mathcal{D}}_j(f,g) = f\Big[\sum_i \overleftarrow{S_+^{(i)}}\tilde{F}(L^2)\frac{(2j+1)(-1)^i\tilde{F}^{-1}(L^2)}{i!(2j+i+1)}\overrightarrow{S_-^{(i)}}\tilde{F}(L^2)\Big]g\,. \tag{2.186}$$

The notation used is explained below. The Casimir operator L^2 on the sphere is given by

$$L^2 = -\frac{\partial^2}{\partial\theta^2} - \cot\theta\frac{\partial}{\partial\theta} - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\ , \tag{2.187}$$

$$L^2 Y_{lm}(\vec{n}) = l(l+1)Y_{lm}(\vec{n})\,. \tag{2.188}$$

The function $\tilde{F}$ is not specified - it can be any function that satisfies

$$\tilde{F}(L^2)Y_{lm}(\vec{n}) = \sqrt{(2j+l+1)!(2j-l)!}\ Y_{lm}(\vec{n}) \tag{2.189}$$

and the explicit form can be ignored when particular calculation is performed. Finally we have

$$S_\pm^{(i)} = \prod_{k=0}^{i-1}\left(k\cot\theta - \frac{\partial}{\partial\theta} \mp \frac{i}{\sin\theta}\frac{\partial^2}{\partial\theta^2}\right)\ . \tag{2.190}$$

The arrows in (2.186) indicate which function is affected by which differential operator, i.e. the direction of the action of the derivatives.

Physical application and examples

Now that we ensured that a $*$-product on the sphere S^2 actually exists let us return to our physical problem. How does spin appear from this program?

In deformation quantization we expect that the Stratonovich-Weyl symbols of the spin to satisfy a relation analogous to their operator counterparts:

$$J_x * J_x + J_y * J_y + J_z * J_z = j(j+1)\,. \tag{2.191}$$

Let us check this property using the explicit forms of the symbols and the $*$-product. The first step is to find the symbols J_i in terms of θ and ϕ. We can write the z-component in the basis in which its diagonal $\hat{J}_z = \sum_{m=-j}^{j} m|jm\rangle\langle jm|$. It follows directly from (2.169) and (2.161) that $Z^j_{rs}(\vec{n}) = (\mathcal{W}(|js\rangle\langle jr|))(\vec{n})$ and therefore, in terms of the matrix elements Z, we write

$$J_z = \sum_{m=-j}^{j} m Z^j_{mm}(\vec{n})\,. \tag{2.192}$$

The diagonal matrix elements can be written simply in terms of the Legendre polynomials:

$$Z^j_{mm}(\vec{n}) = \sum_{l=0}^{2j} \frac{2l+1}{2j+1} C^{j\ j\ l}_{m\ 0\ m} P_l(\cos\theta)\,. \tag{2.193}$$

To find the explicit form we use that the Clebsch-Gordan coefficients satisfy orthogonality relations and we insert $C^{j\ 1\ j}_{m\ 0\ m} = 3m/(2j+1)\sqrt{j(j+1)}$ into the previous equation. Similarly we can find J_x and J_y:

$$J_z = \sqrt{j(j+1)}\cos\theta\,, \tag{2.194}$$

$$J_x = \sqrt{j(j+1)}\sin\theta\cos\phi\,, \tag{2.195}$$

$$J_y = \sqrt{j(j+1)}\sin\theta\sin\phi\,. \tag{2.196}$$

Now before we find the $*$-products in (2.189) we need to point out the orthogonality condition for the Z-functions that follow directly from the properties of the operator kernel:

$$\frac{2j+1}{4\pi}\int_S^2 d\vec{n} Z^j_{rs}(\vec{n}) = \delta_{rs}, \quad \frac{2j+1}{4\pi}\int_S^2 Z^j_{rs}(\vec{n}) Z^j_{pq}(\vec{n}) = \delta_{rq}\delta_{sp}. \tag{2.197}$$

With these we can now write the $*$-products between Z-functions and of J_z with

Z-functions:

$$Z^j_{rs} * Z^j_{pq} = \delta_{sp} Z^j_{rq}, \qquad J_z * Z^j_{rs} = r Z^j_{rs}, \qquad Z^j_{rs} * J_z = s Z^j_{rs}. \tag{2.198}$$

As in (2.195) we incorporate the Clebsch-Gordan coefficients using that

$$C^{j\ 2\ j}_{m\ 0\ m} = [3m^2 - j(j+1)]\sqrt{j(j+1)(2j-1)(2j+3)} \tag{2.199}$$

in order to take advantage of the orthogonality properties. It is straightforward using (2.198) to calculate the $*$-products for all the components

$$J_z * J_z = \frac{j(j+1)}{3} + \frac{3m^2 - j(j+1)}{2j(j+1)(2j-1)(2j+3)}(\cos^2\theta - 1/3)\,, \tag{2.200}$$

$$J_x * J_x = \frac{j(j+1)}{3} + \frac{3m^2 - j(j+1)}{2j(j+1)(2j-1)(2j+3)}(\sin^2\theta\cos^2\phi - 1/3)\,, \tag{2.201}$$

$$J_y * J_y = \frac{j(j+1)}{3} + \frac{3m^2 - j(j+1)}{2j(j+1)(2j-1)(2j+3)}(\sin^2\theta\sin^2\phi - 1/3)\,. \tag{2.202}$$

Adding all the terms together will reproduce (2.191) as we hoped. Having a physically sensible $*$-product on the sphere allows the deformation quantization of particles in spin. Star-exponential, $*$-eigenvalue equations, etc. can be defined as in the previous sections. The j-spin particle will evolve along the classical trajectories as in the bosonic case, at least for a Hamiltonian of the type $H \propto \vec{B}(t)\cdot\vec{J}$.

As a conclusion let us point out that this method can be generalized to other groups of interest. The arguments leading to the choice of S^2 are valid in the case when $SU(2)$ is replaced by a different Lie group as in [39]. Recall that we consider other manifolds besides $\mathbb{R}^{2n}$ as phase spaces, for example when we deal with systems with constraints. In a sense we only identify the right phase space for the spin particle and do not need to introduce additional structures to describe spin. However we have to deal with curved spaces - a feature that can be viewed as a disadvantage.

2.9.2 Quantization using Grassmann variables

Deformation quantization of particles with spin can be done using the same constructs as in the bosonic case, but with Grassmann variables instead. In other words "classical" quantities will be constructed using anticommuting variables – elements of *Grassmann algebra*. This is a situation already encountered in quantum field theory. The path integral approach also requires a "classical" counterparts to the fermionic fields which leads naturally to non-commuting variables. A Grassmann algebra is an algebra with n generators θ_i that satisfy

$$\theta_i\theta_j + \theta_j\theta_i = 0,\ i \neq j = 1, ..., n \ \text{ and } \ \theta_i^2 = 0\,, \tag{2.203}$$

and commute with ordinary numbers. The Grassmann algebra is a graded algebra, where the degree of a monomial is determined by the number of independent generators used in it: $deg(\theta_i) = 1$, $deg(\theta_1\theta_2) = 2$, etc. We can construct a $2n+1$-dimensional linear space where a distinguished basis is

$$1, \quad \theta_1, ..., \theta_n, \quad \theta_{i_1}\theta_{i_2}, \quad \theta_{i_1}\theta_{i_2}\theta_{i_3}, \quad \theta_1...\theta_n\,. \tag{2.204}$$

Therefore we can write a generic function of Grassmann variables as the polynomial:

$$f(\theta) = 1 + \sum_{i=1}^{n} f_i\theta_i + \sum_{i,j=1}^{n} f_{ij}\theta_i\theta_j + ... + f_{1,...,n}\theta_1...\theta_n\,, \tag{2.205}$$

with completely antisymmetric coefficients. As a consequence we cannot have a function of Grassmann variables that is not a polynomial since a formal Taylor series will terminate once the degree of a monomial exceeds n, because of repetitions of at least one θ_i.

Differentiation is defined purely algebraically using the simple rules

$$\frac{\partial}{\partial\theta_i}\,\theta_i = 1\,, \quad \frac{\partial}{\partial\theta_i}\,\theta_j = 0\,,\ (i \neq j) \tag{2.206}$$

and additivity. Since we need to anticommute the variables in order to bring them to the derivatives corresponding to them we write a generalized Leibniz rule

$$\frac{\partial}{\partial\theta_i} f_1 f_2 = \frac{\partial f_1}{\partial\theta_i} f_2 + (-1)^{deg(f_1)} f_1 \frac{\partial f_2}{\partial\theta_i}\,. \tag{2.207}$$

Similarly we define integration on the simplest elements

$$\int d\theta_i = 0\,, \qquad \int \theta_i d\theta_i = 1 \tag{2.208}$$

and use the additivity property to generalize to generic polynomials. It is easy to see that integration and differentiation (up to a minus sign) are in fact the same operation.

Wigner-Weyl correspondence

In deformation quantization we need a set of Grassmann variables π_i, $i = 1, ..., n$, that correspond to the momenta. Also we assume that the program we followed for bosons is going to be the same for fermions. Indeed there is a Wigner-Weyl correspondence and a $*$-product for functions of Grassmann variables with the desired properties. Standard operator quantization for fermions replaces commutators for creation and annihilation operators with anti-commutators. We can define symbols of the Fermi operators using Fourier transform

$$\tilde{f}(\xi,\zeta) = \int f(\theta,\pi)\, e^{-i\theta\xi - i\pi\zeta} d\theta d\pi\,, \tag{2.209}$$

$$f(\theta,\pi)=\int \tilde{f}(\xi,\zeta)\, e^{i\theta\xi+i\pi\zeta} d\theta d\pi\,, \tag{2.210}$$

where $d\theta = d\theta_1, ..., d\theta_n$ and $\theta\xi = \sum_{i=1}^{n} \theta_i \xi_1$, etc. Then the Weyl map for fermionic degrees of freedom is defined as in (2.19) via the Fourier transform (2.209) and (2.210)

$$\hat{f}=\int f(\theta,\pi)\, e^{i(\hat{\theta}-\theta)\xi+i(\hat{\pi}-\pi)\zeta} d\theta d\pi d\xi d\zeta\,. \tag{2.211}$$

We can identify the Stratonovitch-Weyl kernel or *quantizer* from the above

$$\hat{w}(\theta,\pi)=\int e^{i(\hat{\theta}-\theta)\xi+i(\hat{\pi}-\pi)\zeta} d\theta d\pi\,. \tag{2.212}$$

Similarly to the Stratonovich method we can now invert the Weyl map to get the Wigner transform:

$$f(\theta,\pi)=\mathrm{Tr}\left[\hat{f}\hat{w}(\theta,\pi)\right]. \tag{2.213}$$

The Wigner function is again defined to be proportional to the symbol of the density operator.

The $*$-product of two symbols $f * g$ can be found as in the bosonic case, using the Wigner-Weyl correspondence to relate it to $\hat{f}\hat{g}$. From this we can derive an integral representation and then using Taylor series to get the pseudo-differential form. However free from the complications of the curved phase space in Stratonovich method, the Grassmann variable method is so close to the bosonic case that we can simply guess the correct form of the $*$-product:

$$f * g = f \exp\left\{\frac{i\hbar}{2}\left(\overleftarrow{\partial}_\theta\overrightarrow{\partial}_\pi + \overleftarrow{\partial}_\pi\overrightarrow{\partial}_\theta\right)\right\} g\,. \tag{2.214}$$

We have used the exponentiation of the Grassmann-variable Poisson bracket as a

definition similarly to equation (2.28)

$$\{f,g\}_F = \sum_{i=1}^{n}\left(\frac{\partial f}{\partial\theta_i}\frac{\partial g}{\partial\pi_i}+\frac{\partial f}{\partial\pi_i}\frac{\partial g}{\partial\theta_i}\right). \tag{2.215}$$

A systematic derivation of this $*$-product can be found in [40]. However we will simply provide the integral representation as a reference:

$$f*g = -\frac{\hbar^2}{4}\int f(\theta_1,\pi_1)g(\theta_2,\pi_2)e^{-\frac{2i}{\hbar}[\pi(\theta_1-\theta_2)+\pi_1(\theta_2-\theta)+\pi_2(\theta-\theta_1)]}d\pi_1 d\theta_1 d\pi_2 d\theta_2\,. \tag{2.216}$$

Example

Let us now see how can this quantization technique works for a simple system. Following Berezin and Marinov (see [7]) for a non-relativistic spin we can write the Hamiltonian in the form:

$$H(\theta,\pi) = -i\omega\theta_1\theta_2\,. \tag{2.217}$$

The Lagrangian associated to this system is

$$L(\theta,\dot\theta) = \frac{i}{2}(\theta_1\dot\theta_1+\theta_2\dot\theta_2)+i\omega\theta_1\theta_2\,, \tag{2.218}$$

and therefore the canonical momenta are given in terms of θ: $\pi_i = -i\theta_i/2$. Using this expression we can rewrite the Hamiltonian in the form:

$$H(\theta,\pi) = \omega(\theta_1\pi_2-\theta_2\pi_1)\,. \tag{2.219}$$

This expression is proportional to the angular momentum, which corresponds to the spin – $H=\omega S_3$.

As before we can define star-exponentials, $*$-eigen value equations and projectors. While the generalizations turn out to be almost identical to the bosonic case, the derivations are quite interesting, so one can refer to [7], [41],[40] and [45] for the full

detail. For our purposes we will only need the star-exponentials in order to find the states and the corresponding energies:

$$Exp_*(tH) = \rho_{1/2} e^{-it\omega/2} + \rho_{-1/2} e^{-it\omega/2} \,. \tag{2.220}$$

Where the states and the energies are given by

$$\rho_{\pm 1/2} = 1/2 \mp i\theta_1\theta_2/\hbar, \qquad E_{\pm 1/2} = \pm\omega/2 \,. \tag{2.221}$$

One can now find the projections of the spin and their average values, the Moyal equations of motion for the Wigner function and the spin, etc.

The Grassmann variable method presents an algebraic version of spin quantization. While it lacks the geometric insight of the Stratonovich quantization, it is simpler and the resemblance with the bosonic case is obvious. Also, unlike the Stratonovich formulation, the connection with quantum field theory is direct. That relationship is exploited in the $*$-product formulation of quantum field theory – an active and interesting field of research. However that is outside of the scope of this work

Chapter 3

Contact interactions

In this chapter we will address the problems associated with point interaction and reflective walls, i. e. contact interactions. We will refer to interactions as contact interactions whenever they are described with a potential with discontinuities. As mentioned earlier deformation quantization requires smooth potentials when the pseudodifferential form of the equations are used[1] or integrable ones in the case of the integral form of the equations. Either way a potential like the infinite wall or infinite step presents a certain challenge. At first glance they cannot be treated in deformation quantization. However their importance demands a solution in the deformation quantization framework. More generally, infinite potentials need to be included in deformation quantization. Here we present possible resolutions of that problem.

3.1 The problem with sharp potentials

Sharp potential features are tricky in phase space. The vanishing width of point interactions and reflecting walls results in discontinuous classical phase-space trajectories. The quantum situation seems better. In operator quantum mechanics, phase space is not central, and one only needs to impose appropriate boundary conditions

[1] We can allow distributions to be used in order to include more potentials

on wave functions in coordinate space. The boundary conditions conserve probability and can be understood as necessary for self-adjointness of Hermitian operators, like the Hamiltonian, or extensions thereof.[2]

However, if one insists on doing quantum mechanics in phase space (or deformation quantization) with sharp potential features, the problem is not as easily fixed [29, 54, 30, 55, 31]. The $*$-eigenvalue equations are defined only for smooth potentials. At least in principle, for sharp but finite potentials this problem can be dealt with, since they are integrable and the integral form of the $*$-product is defined. However that is not applicable when infinite potentials are involved, the reason being that the formal expression for the $*$-product is not convergent. Here we will investigate this phenomenon, in both phase-space quantum mechanics and Schrödinger wave mechanics. We believe that such extreme examples can tell us something interesting. For simplicity, we will restrict attention to the non-relativistic quantum mechanics of a single particle, moving in one spatial dimension.

Arguably, the simplest example of a sharp potential feature that illustrates the problem of interest is an infinite potential wall. Equivalently, we can consider a particle restricted to the half-line. In either case, however, the dynamics that is important for us is sharp, i.e. it takes place at a single point. The corresponding potential has a feature of vanishing width, $w = 0$, or infinite sharpness, $\alpha := 1/w = \infty$.

A remarkable phenomenon helps us to understand the origin of the complications in phase-space quantum mechanics brought about by sharp potential features [75]. For particle energy exceeding a discontinuous potential, so-called non-Newtonian scattering occurs [10]. Quantum mechanically, there is a non-zero probability of reflection off the sharp feature, even though the process does not occur classically.[3] Most strik-

[2] See [11] for nice expositions of the theory of self-adjoint extensions, and [17] for intriguing properties of contact interactions.

[3] It should be noted, however, that this is a *wave* phenomenon, and so will be present in the Koopman-von Neumann operator formulation of classical mechanics. In the presence of sharp po-

ingly, the probability is independent of Planck's constant, and so does not vanish as $\hbar \to 0$.

This indicates that the zero-width limit ($w \to 0$) and the classical limit ($\hbar \to 0$) do not commute. This non-commutativity of limits is hard to incorporate into phase-space quantum mechanics, or deformation quantization. Recall that in it, the algebra of quantum observables is realized as an $\hbar$-deformation of the classical one in phase space. Non-Newtonian scattering cannot be described by simply $\hbar$-deforming canonical classical mechanics.

Dias and Prata [29] confronted this problem in phase-space quantum mechanics, for the special case of Dirichlet boundary conditions for the Schrödinger wave functions. To describe the complication they found, recall that the Wigner function $\rho(q,p)$ is the central object in phase-space quantum mechanics (see section 4 below, and [79, 43], e.g.). At finite α, it can be found two ways. First, one can start from the wave functions $\psi(q)$, and build the corresponding density operator. Then a Wigner transform will yield the Wigner function; denote the result $\rho_\alpha[\psi](q,p)$. Alternatively, one can use the dynamical equations of phase-space quantum mechanics. The $*$-eigenvalue equations can be solved, with a solution we denote by $\rho_\alpha[*](q,p)$. As long as $\alpha < \infty$, we must have

$$\rho_\alpha[\psi](q,p) \;=\; \rho_\alpha[*](q,p) \;. \tag{3.1}$$

Dias and Prata treated the case $\alpha = \infty$, and found

$$\rho_\infty[\psi](q,p) \;\neq\; \rho_\infty[*](q,p) \;. \tag{3.2}$$

They assumed that the Wigner transform $\rho_\infty[\psi](x,p)$ was physical and added a boundary potential so that the $*$-eigenvalue equations were compatible. That is,

tential features, then, the latter formulation is not equivalent to the canonical one.

they modified the $*$-eigenvalue equations so that their solutions were $\tilde{\rho}_\infty[*](q,p) = \rho_\infty[\psi](q,p)$.

In an effort to justify their somewhat ad hoc procedure, alternatives to the $*$-eigenvalue equations were found in [54]. Dias and Prata then demonstrated [30] that the use of the alternative, so-called $*$-eigen-$*$ value equations, had a certain equivalence to their treatment. Since the $*$-eigen-$*$ value equations were derived, rather than postulated, those arguments provided an indirect justification of their procedure.

A more direct argument can follow by noting that zero-width (or sharp) features must be understood fundamentally as $\alpha \to \infty$ limits of nonzero-size (smooth) ones. That is, the sharp case is an idealization, whose treatment should provide a shortcut to the results obtained in the physical limit.

In that spirit, the infinite potential wall was described by a limit of the Liouville potential in [30]. There it was shown that the Wigner transform of the wave functions with Dirichlet boundary conditions was indeed physical, as was assumed by Dias and Prata [29]. That is,

$$\lim_{\alpha\to\infty} \rho_\alpha[\psi](q,p) \;=\; \lim_{\alpha\to\infty} \rho_\alpha[*](q,p) \;=\; \rho_\infty[\psi](q,p)\ . \tag{3.3}$$

The first equality was guaranteed, by (3.1), but the second was not. If the limit had produced $\rho_\infty[*](q,p)$ instead, for example, then the Wigner transform would have had to be modified, rather than the $*$-eigenvalue equations.

Dirichlet boundary conditions are only a special case of the possible Robin (or mixed) boundary conditions, studied in [75], however. In this work, we will extend the result of [55] to the general case of Robin boundary conditions.

We should also mention that in [55], the connection was first made between self-adjoint extensions of the Hamiltonian and the problem (3.2) found by Dias and Prata

[29]. Subsequently, those authors were able to show that the Hamiltonians that included the boundary potentials they introduced were indeed self-adjoint [31].

We will first present in more detail the Kryukov-Walton $*$-eigen-$*$ equations, followed by an outline of Dias and Prata's work. A short overview of non-standard walls is provided to clarify the connection between boundary condition, operator extensions and physics. Finally we will present in full how, at least for the infinite wall, the problems associated with sharp features can be handled using the Morse potential as in [5].

This last problem is essentially the core of this chapter. Robin boundary conditions for wave functions are derived by taking a limit of a piece-wise flat potential, following [68, 38]. There, mass-dependent fine tuning of the potential is necessary to realize a non-standard wall, i.e. to avoid the standard Dirichlet boundary conditions. We point out that this fine tuning is equivalent to selecting a reflection resonance, as defined in [12].

Instead of just explaining the one sharp potential feature of an infinite wall, however, a discontinuous piece-wise flat potential introduces more. An analogous calculation is carried out for a smooth Morse potential. The Robin boundary conditions are recovered, again with the same kind of mass-dependent fine tuning already found in [68, 38]. In the smooth case, we also show that reflection resonances are again selected.

We also consider Wigner functions for the Morse potential are considered. The $*$-eigenvalue equations they obey are converted to difference equations by a Mellin transform and the solutions are found. In section 5, the Wigner transform of the Morse wave functions is performed. Also the general solution to the $*$-eigenvalue equations is written and shown to be the same as the corresponding Wigner transforms. Most importantly, we show that in the appropriate limit, those Wigner functions reduce to the expected ones [75].

3.2 Deformation quantization techniques for contact interactions

In this section we consider two equivalent independent methods treating the infinite wall potential. We modify the equations of motion of deformation quantization, keeping the Hamiltonian intact or equivalently we change the form of the Hamiltonian in order to conserve the form of the dynamical equations. In both methods we modify the dynamics in order to allow deformation quantization treatment of the infinite wall.

3.2.1 Dias-Prata method

In [29] Dias and Prata consider the infinite well in deformation quantization by changing the equations of motion for the Wigner function and the boundary conditions associated with them. We provide a short summary of some of the important results.

There are two ways of approaching the problem of a particle confined on a finite interval $[a, b]$. One is to solve in the bulk and then impose boundary conditions from physical consideration while keeping the wave function identically zero outside of the bulk. This is shown not to work in deformation quantization since the non-locality in the dynamical equations results in nontrivial effects on the boundaries. The Wigner functions defined from the corresponding wave functions via the Wigner transform do not satisfy the $*$-eigenvalue equations on the bulk [29].

Alternatively, we can introduce a potential that accounts for the boundaries and consider a system without constraints. That recipe is more suited to be applied for Wigner functions. Using the connection with operator quantum mechanics Dias and Prata derive a boundary correction to the bulk Hamiltonian along with the relevant boundary conditions.

Let us consider the pure state wave function $\psi(q) = \langle q|\psi\rangle$, with $|\psi\rangle$ an eigenvector

of the bulk Hamiltonian H. The Baker function will satisfy

$$\psi^*(q-y)\psi(q+y) = 0 \quad \text{unless} \quad a < q-y < b \quad \text{and} \quad a < q+y < b. \tag{3.4}$$

Defining auxiliary Wigner functions via

$$\rho_1(q,p) = \lim_{\epsilon \to a+0} \frac{1}{\pi\hbar} \int_{q-\epsilon}^{\epsilon-q} dy e^{-2ipy/\hbar} \psi^*(q-y)\psi(q+y)\,, \tag{3.5}$$

$$\rho_2(q,p) = \lim_{\epsilon \to b-0} \frac{1}{\pi\hbar} \int_{\epsilon-q}^{q-\epsilon} dy e^{-2ipy/\hbar} \psi^*(q-y)\psi(q+y)\,, \tag{3.6}$$

we can use step functions to the left and right of the center of the wall[4]

$$\theta_L(q) = \theta(q-a) - \theta(q-(a+b)/2)\,, \tag{3.7}$$

$$\theta_R(q) = \theta(q-(a+b)/2) + \theta(b-q)\,, \tag{3.8}$$

to express he Wigner function as

$$\rho(q,p) = \theta_L(q)\rho_1(q,p) + \theta_R(q)\rho_2(q,p)\,. \tag{3.9}$$

Dias and Prata show that the Wigner function and $\rho_{1,2}$ satisfy Dirichlet boundary conditions as long as the boundaries are approached from the interior of the interval, since the integrals are improper and the boundary conditions are defined as limits as the argument approaches a and b.[5] In fact the boundary conditions do not affect the Wigner function but the derivatives only. For example for wave functions satisfying

[4]The step function $\theta_L(q) = 1, \quad q \in (a,(a+b)/2)$ and 0 otherwise. Analogously for the right side of the interval we can define $\theta_R(q)$

[5]We will show later that this result is true in general but other, more general boundary conditions are also admissible in certain cases.

Dirichlet boundary conditions (realized as limits) we get

$$\lim_{\epsilon\to 0}\partial_q\rho(a+\epsilon,p)=\lim_{\epsilon\to 0}\partial_q\rho(b-\epsilon,p)=0. \tag{3.10}$$

The result (3.9) allows us to determine the boundary terms that complement the bulk Hamiltonian in order to recover the Wigner functions using Wigner-Weyl correspondence. One has to point out that we assume the Wigner-Weyl correspondence is unchanged by the boundary effects. This will be shown to be true in the later sections. We get the following "corrected" $*$-eigenvalue equation

$$H*\rho(q,p)-\frac{\hbar^2}{2m}\delta'(q-a)*\rho(q+\epsilon,p)+\frac{\hbar^2}{2m}\delta'(q-b)*\rho(q-\epsilon,p)=E\rho(q,p)\,. \tag{3.11}$$

This construction provides a better understanding of the contact interactions at least for infinite well. However it is difficult to apply in general for particular calculations and other potentials with sharp features. Also ultimately the Shrödinger equation and the Wigner-Weyl correspondence are at the base of this argument. This is why a motivation that comes from within deformation quantization is desirable, also one that is easier to implement in practice. Another question arises – it is known that Dirichlet boundary conditions are not the only admissible boundary conditions in operator quantum mechanics. Is it then possible to recover more general boundary conditions using different method?

3.2.2 The $*$-eigen-$*$ equations

In this section we show that starting with a conveniently chosen smooth potential one can derive an equation to substitute the $*$-eigenvalue equation in the case of sharp potentials constructed by walls and delta functions.

Let us consider an infinite wall. We will pick the Liouville potential $H_L=p^2+e^{2\alpha q}$, ($m=1/2$ for simplicity) and take the limit $\alpha\to\infty$ to recover an infinite wall. The

Wigner function for this potential can be shown to satisfy a fourth order differential equation in that limit:

$$\partial_q^4\rho(q,p)/16 + (p^2+E)\partial_q^2\rho(q,p)/2 + (p^4 - 2k^2p + k^4)\rho(q,p) = 0. \tag{3.12}$$

The equation can be written in terms of the free particle Hamiltonian

$$(p^2 - E) * \rho(q,p) * (p^2 - E) = 0. \tag{3.13}$$

This equation is called $*$-eigen-$*$ equation and turns out ([54]) to be relevant to wider class of potentials. Choosing the potential

$$H_\alpha = p^2 + e^{-2\alpha(q+1)} + e^{2\alpha(q-1)}\,, \tag{3.14}$$

allows us to recover the infinite well potential in the limit $\alpha \to 0$. In [54] one can see that in the large α limit one recovers the same equation (3.12) as for the infinite wall potential. In other words in the bulk where the particle is free the $*$-eigenvalue equation does not hold – instead (3.12) is satisfied. Kryukov and Walton show the same result for the case when the potential is a delta function (analogously recovered as a limit of an exponential function).

More generally one can write a potential that is a sum of walls, delta functions and a regular function $V(x)$ and ask the same question. What is the equation that replaces the $*$-eigenvalue equation? For the infinite wall one finds

$$\begin{aligned}\frac{1}{16}\partial_q^4\rho + \frac{1}{2}(p^2+E)\partial_q^2\rho + (p^4 - 2k^2p + k^4)\rho + (p^2-E)\mathrm{Re}(V*\rho) - \\ p\,\partial_q\mathrm{Im}(V*\rho) - \frac{1}{4}\partial_q^2\mathrm{Re}(V*\rho) - \mathrm{Im}(V*p\,\partial_q\rho) + \mathrm{Im}[V*\mathrm{Im}(V*\rho)] + \\ \mathrm{Re}[V*\mathrm{Re}(V*\rho)] + \mathrm{Re}\left[V*\left(p^2\rho - E\rho - \frac{1}{4}\partial_q^2\rho\right)\right] = 0\,.\end{aligned} \tag{3.15}$$

This may look very complicated but it can be written as a $*$-eigen-$*$ equation for the bulk Hamiltonian (away from the wall) – $H = p^2 + V(q)$

$$(H(q,p) - E) * \rho(q,p) * (H(q,p) - E) = 0\,. \tag{3.16}$$

as shown in [75]. The $*$-eigen-$*$ equation can be further generalized when non-stationary states are involved. Also it is still valid for a theta-function potential, where the the potential is sharp but finite.

Finally (3.16) can be used for Hamiltonians of the form

$$H = p^2 + \theta(q)q^2\,. \tag{3.17}$$

In other words, when we match two potentials without sharp features

$$V_- = 0, \quad q < 0 \text{ and } V_+ = q^2, \quad q > 0\,, \tag{3.18}$$

having discontinuity at the first or higher order derivatives. Dias and Prata showed certain equivalence between those two methods. Also the second method in a sense justifies the first since it is derived within deformation quantization and from first principles.

To conclude let us point out that the Liouville potential used to recover the walls always produces Dirichlet boundary conditions, i. e. *standard walls*. However non-standard wall are physical and need to be included. We will consider nonstandard walls in operator quantum mechanics in the next section.

3.3 Non-standard walls. Self-adjoint extensions and their physical significance

An infinite potential wall where the Dirichlet boundary conditions are imposed on the wave function is called a *standard wall*. We are concerned with is the *non-standard* walls which include the Neumann boundary conditions and more general Robin boundary conditions. The latter are a linear combination of Dirichlet and Neumann, so they include them as particular cases

$$\psi(0) + L\psi'(0) = 0\,. \tag{3.19}$$

We will show that non-standard walls arise naturally. They have physical interpretation and not considering them may result in overlooking important physics.

Let us consider the infinite well as treated by [14]. An infinitely deep potential well is equivalent to a free particle confined on the interval $-a \leq x \leq a$. The energy and momentum, in coordinate representation, are given by the operators

$$\hat{H} = \hat{p}^2/2m, \quad \hat{p} = -i\hbar\frac{\partial}{\partial q}\,. \tag{3.20}$$

We are used to assume that observables are self-adjoint operators, however that statement can be misleading and even wrong. In order an operator to be self adjoint, its domain must coincide with the domain of the adjoint operator, a condition that is very often neglected. Let us clarify with the following example

$$(f, \hat{p}\, g) - (\hat{p} f, g) = \int_{-a}^{a} dq(\bar{f}\hat{p}(g) - \overline{\hat{p}(f)}g) = -i\hbar\left[\overline{f(a)}g(a) - \overline{f(-a)}g(-a)\right], \tag{3.21}$$

the operator $\hat{p}$ is self-adjoint only if we demand that two arbitrary wave functions

$f(q)$ and $g(q)$ satisfy the condition

$$[f(a)/f(-a)]^* = g(-a)/g(a)\,. \tag{3.22}$$

Therefore all functions that are included in the domain of $\hat{p}$ are of the form

$$f(a) = e^{-2i\pi\alpha} f(-a), \qquad \alpha \in [0,1)\,. \tag{3.23}$$

This simply means that not all functions on the interval $x \in [-a, a]$ can be taken as wave functions. For every α there will be a different set of admissible wave functions and therefore α parametrizes a family of possible domains for the operator $\hat{p}$ formally given by (3.20). The difference between the definitions of symmetric and self-adjoint operators now proves to be significant, since every domain defined by (3.23) defines a different self-adjoint extension of the momentum. Not only is the self- adjoint extension is not unique, but we find infinitely many extensions instead.

Now to show that this is not just of purely mathematical interest let us present Capri's example [14]. We pick a domain corresponding to $\alpha = 1/2$, i.e. twice differentiable anti-periodic functions with eigenstates and spectrum given by

$$f_n(q) = \frac{e^{i\pi(n+1/2)q/a}}{\sqrt{2a}}\,, \qquad p_n = \frac{\pi\hbar(n+1/2)}{a}\,. \tag{3.24}$$

The same states are eigenstates for the Hamiltonian except that all the eigenvalues are doubly degenerate:

$$\begin{aligned} \hat{H} f_n(q) &= \pi^2\hbar^2(n+1/2)^2/2ma^2 f_n(q)\,, \\ \hat{H} f_{1-n}(q) &= \pi^2\hbar^2(n+1/2)^2/2ma^2 f_{1-n}(q)\,. \end{aligned} \tag{3.25}$$

The ground states are not eigenstates for the parity and time reversal operators. Since

they commute with the Hamiltonian but do not leave the ground states invariant those are spontaneously broken symmetries. If we attempt to restore those symmetries by taking linear combination of the ground states, the new ground states are not translationally invariant since they are not eigenstates of the momentum.

A one-dimensional crystal with alternating atoms we will have boundary conditions that are periodic from a fixed atom to its next nearest neighbor. Therefore the nearest neighbor can have anti-periodic boundary condition. That is why the states are not translationally invariant or time/position reversal invariant.[6]. This simple example shows how different self-adjoint extensions can describe different physics. Therefore it is important to consider the Robin boundary conditions and not just from a mathematical point of view.

How can we determine if a self-adjoint extension of the operator exists and if it does is it unique or there are many of them as in the case of the momentum operator for infinite well? A theorem by Weyl generalized by von Neumann answers that question (see [11]).

Let us define the *deficiency subspaces* $\mathcal{N}_\pm$ of an operator $\hat{A}$

$$\mathcal{N}_+ = \{\psi \in \mathcal{D}(\hat{A}^\dagger)\,, \quad \hat{A}^\dagger\psi = z_+\psi\,, \quad \mathrm{Im}z_+ > 0\}\,, \tag{3.26}$$

$$\mathcal{N}_- = \{\psi \in \mathcal{D}(\hat{A}^\dagger)\,, \quad \hat{A}^\dagger\psi = z_-\psi\,, \quad \mathrm{Im}z_- < 0\}\,, \tag{3.27}$$

where $\mathcal{D}(\hat{A}^\dagger)$ is the domain of $\hat{A}^\dagger$. The dimensions of those spaces are called *deficiency indices* of the operator A and they are denoted by (n_+, n_-), $dim(\mathcal{N}_\pm) = n_\pm$. The deficiency indices, therefore, do not depend on the particular representative $z_\pm$ and can be simply chosen to be $\pm i\lambda$ with arbitrary $\lambda > 0$.

Von Neumann theorem: a necessary and sufficient condition for an operator $\hat{A}$ with deficiency indices (n_+, n_-) to have

[6]For further detail see [14]

1.) an unique self-adjoint extension is $n_+ = n_- = 0$. In other words the operator is self-adjoint.

2.) infinitely many self-adjoint extensions is $n_+ = n_- > 0$. The self adjoint extensions are parametrized by an $n \times n$ matrix, where $n_+ = n_- = n$

3.) no self-adjoint extensions is $n_+ \neq n_-$. The operator is not self-adjoint.

That theorem may give us the general answer but finding the self-adjoint operator is not trivial. For examples see [14] and [11]. In those papers several nontrivial examples are available.

In the case we are interested in – particle on the half line – the possible extensions of the Hamiltonian exist only if the Robin boundary condition exist and they are parametrized by a single parameter. We will discuss that in more detail later.

3.4 Robin boundary conditions from a discontinuous potential

Consider a non-relativistic quantum particle that is confined to the positive half-line with coordinate x, but is otherwise free. Its wave function must satisfy the Robin boundary conditions

$$\psi(0) \; + \; L\,\psi'(0) \; = \; 0 \tag{3.28}$$

for some real length parameter $L \in (-\infty, \infty) \cup \{\infty\}$. The Robin, or mixed boundary conditions generalise the Dirichlet ($L = 0$) and Neumann $L \to \pm\infty$) ones. They conserve probability and realize the self-adjoint extension of the Hermitian Hamiltonian $H = p^2/2m$ on the half-line.

Even though there is no mathematical reason other than simplicity to prefer them, Dirichlet boundary conditions are the most commonly applied. For that reason, infinite walls with other boundary conditions imposed are known as *non-standard*

walls [38].

The real wave function

$$\psi_k(q) \;=\; \sin(kq+\phi) \tag{3.29}$$

obeys the boundary condition (3.28) if the phase is chosen so that

$$kL \;= \tan\phi \;. \tag{3.30}$$

It is appropriate for an unbound particle of energy $\hbar^2k^2/2m$. For the same dynamics, one bound state also exists, with (unnormalized) wave function $e^{-q/L}$ and energy $-\hbar^2/2mL^2$, provided $L>0$.

The bound state provides the length scale L: its energy defines it, and its wave function has range L. This does not work for $L<0$, however. A more democratic interpretation is provided by the Wigner time delay (advance)

$$\delta t \;=\; 2\hbar\,\frac{d\phi}{dE} \;=\; -\,\frac{2mL}{\hbar k(1+k^2L^2)}\;, \tag{3.31}$$

for $L>0$ ($L<0$).[7]

Let us now consider a particle moving on the (whole) real line with coordinate q and Hamiltonian

$$H \;=\; p^2/2m \;+\; V(q)\;. \tag{3.32}$$

A particle with energy $2mE \;=\; \hbar^2k^2$ has a time-independent wave function $\psi(q)$ satisfying the stationary Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(q)}{dx^2} \;+\; V(q)\,\psi(q) \;=\frac{\hbar^2k^2}{2m}\,\psi(q)\;. \tag{3.33}$$

We will show that the Robin boundary conditions can arise from the limit of a smooth

[7] See [38] and references therein.

potential. This generalises the derivation of Dirichlet boundary conditions from the $\alpha \to \infty$ limit of the Liouville potential $V_\alpha(q) = (\hbar^2\kappa^2/2m)\, e^{-2\alpha q}$. In the context of deformation quantization, the latter result was obtained in [55].

To prepare for that calculation, we'll first study a discontinuous, piece-wise flat potential:

$$V_\alpha(q) \;=\; \begin{cases} \infty\,, & q < 0, \\ -\frac{\hbar^2\kappa^2}{2m}\,\alpha\ell\,(\alpha\ell\,+\,1)\;, & 0 \le q < 1/\alpha\;, \\ 0\;, & q > 1/\alpha. \end{cases} \tag{3.34}$$

Here ℓ, $1/\alpha$ and $1/\kappa$ are lengths, with $\kappa^2 > 0$ controlling the overall strength of the potential. Šeba [68] showed that when this potential becomes an infinite wall as $\alpha \to \infty$, Robin boundary conditions are recovered.

To see this, solve the Schrödinger equation piece-wise to get

$$\psi_\alpha(q) \;=\; \begin{cases} 0\;, & q < 0\;, \\ \sin\left(q\sqrt{k^2 + \kappa^2\,\alpha\ell\,(\alpha\ell\,+\,1)}\right), & 0 \le q < 1/\alpha \\ A\,\sin(kq + \phi)\;, & q > 1/\alpha \end{cases} \tag{3.35}$$

for an energy $E = \hbar^2k^2/2m > 0$. Notice that the boundary conditions at $q = 0$ are Dirichlet. Those at $q = 1/\alpha$, however, are of the mixed type, i.e., Robin. We can therefore derive Robin boundary conditions at $q = 0_+ := \lim_{\alpha\to\infty} 1/\alpha$. From the point of view of the physical wave function outside the resulting point interaction, it is the Robin (instead of the Dirichlet) boundary conditions that must be imposed.

Matching the wave-function values and derivatives at $q = 1/\alpha$ gives

$$\sin\left(\frac{1}{\alpha}\sqrt{k^2 + \kappa^2\,\alpha\ell\,(\alpha\ell\,+\,1)}\right) \;=\; A\,\sin(k/\alpha + \phi)\;,$$
$$\sqrt{k^2 + \kappa^2\,\alpha\ell\,(\alpha\ell\,+\,1)}\,\cos\left(\frac{1}{\alpha}\sqrt{k^2 + \kappa^2\,\alpha\ell\,(\alpha\ell\,+\,1)}\right) \;=$$

$$Ak\,\cos(k/\alpha+\phi)\ . \qquad (3.36)$$

For large α, these equations become

$$\begin{aligned} \sin(\kappa\ell) \;&=\; A\,\sin\phi \;+\; \mathcal{O}(\alpha^{-1})\ , \\ \alpha\kappa\ell\,\cos(\kappa\ell) \;+\; \frac{\kappa}{2}\,\cos(\kappa\ell) \;-\; \frac{\kappa^2\ell}{2}\,\sin(\kappa\ell) \;&=\; Ak\,\cos\phi \;+\; \mathcal{O}(\alpha^{-1})\ . \end{aligned} \qquad (3.37)$$

Clearly, the order α term in the second equation must vanish, so that $\cos(\kappa\ell)=0$, implying

$$\kappa \;=\; \kappa_n := \;\frac{\pi}{\ell}\left(n+\frac{1}{2}\right)\ ,\quad n\in\mathbf{Z}\ . \qquad (3.38)$$

Then $\sin(\kappa_n\ell)=(-1)^n$, and we find

$$A \;=\; A_n \;:=\; \sqrt{1+\frac{\pi^4(n+\frac{1}{2})^4}{4k^2\ell^2}}\ ,\qquad \tan\phi \;=\; \tan\phi_n \;=\; -\frac{2k\ell}{\pi^2(n+\frac{1}{2})^2}\ . \qquad (3.39)$$

Comparing to (3.30), we get

$$L \;=\; L_n \;:=\; \frac{2\ell}{\pi^2(n+\frac{1}{2})^2} \qquad (3.40)$$

for the Robin length scale.

So the Robin boundary conditions are found for $q=0_+$, but only barely: there are solutions only for a discrete set of values of κ, indexed by the integer n. The strength of the potential needs to be finely tuned, tuned differently for different particle masses,[8] and the non-standard Robin boundary conditions arise for a very limited subset of possible parameters.

What is the physical significance of the fine tuning? It selects a resonance. Although for this potential the probability of reflection is always one, a reflection resonance can still be defined, by a rapid change of π in the phase shift [12]. From the

[8] For the standard wall with Dirichlet boundary conditions, this mass dependence is not present.

matching conditions (3.36) we can derive

$$\frac{\tan(j/\alpha)}{j/\alpha} \;=\; \frac{\tan(k/\alpha+\phi)}{k/\alpha}\;, \tag{3.41}$$

where $j := [k^2+\kappa^2\alpha\ell(\alpha\ell+1)]^{1/2}$. Demanding that $0=\frac{d^2\phi}{dk^2}$, and selecting the maxima of $\frac{d\phi}{dk}$, leads to $\tan(j/\alpha)=\infty$, or

$$\frac{j}{\alpha} \;=\; \frac{[k^2+\kappa^2\alpha\ell(\alpha\ell+1)]^{1/2}}{\alpha} \;=\; \left(n+\frac{1}{2}\right)\pi\;, \quad n\in\mathbb{Z}\;\;. \tag{3.42}$$

In the $\alpha\to\infty$ limit, the fine-tuning condition (3.38) is recovered.

Let us note that the reflection resonance condition (3.42) corresponds to Neumann boundary conditions at $q=1/\alpha$, even before the $\alpha\to\infty$ limit is taken. Of course, the requirement (3.38) for Robin boundary conditions does not select Neumann boundary conditions. Substituting (3.38) yields

$$\frac{j}{\alpha} \;=\; \left(n+\frac{1}{2}\right)\pi \;+\; (\alpha L_n)^{-1} \;+\; \mathcal{O}(\alpha^{-2})\;\;, \tag{3.43}$$

using (3.40). This shows that the fine tuning is to near a reflection resonance; how it is approached in the $\alpha\to\infty$ limit determines the Robin length scale L_n and so the boundary condition that is realized.

Let us also consider the bound states of the Šeba potential in the $\alpha\to\infty$ limit. For the negative energy states the wave function will decay exponentially in the interval $q\in(1/\alpha,\infty)$. Therefore the right hand sides of the matching conditions (3.36) will be replaced by their exponential versions. In general we can find the discrete energies as solutions to a transcendental equation following from the matching conditions. The exact energies, therefore, cannot be written in closed terms. Luckily, we only need to determine them for $\alpha\to\infty$. Dividing the matching conditions for the wave function

and its derivative yields

$$\sqrt{-2m|E|/\hbar^2 + \kappa^2\,\alpha\ell\,(\alpha\ell\,+\,1)}\,\cot\left(\frac{1}{\alpha}\sqrt{-2m|E|/\hbar^2 + \kappa^2\,\alpha\ell\,(\alpha\ell\,+\,1)}\right) \;=\; -\sqrt{2m|E|/\hbar^2}\;. \tag{3.44}$$

As before we can compare the coefficients in front of the different powers of α. The only possible energy is then $E = -\hbar^2\kappa^4\ell^2/8m$. Taking into account that (3.38-3.40) are needed for the Robin boundary conditions to arise, we obtain the correct energy $-\hbar^2/2mL^2$ in the $\alpha \to \infty$ limit. The bound state energy is recovered from the Šeba potential, for $L > 0$. We can also verify that, for the same values of the parameters, the (unnormalized) wave function of the unique bound state is $e^{-q/L}$ in the limit.

One criticism of these results could be that Dirichlet boundary conditions were assumed, not derived for the infinite wall (with no extra structure) at $x = 0$ in the Šeba potential. In addition, infinite potential walls are only idealisations of very high, but finite walls, and so the infinite wall should be treated as the limit of a finite wall. However, similar results were obtained later in [38] but with a finite wall, and no particular boundary conditions assumed. Robin boundary conditions were again obtained, with non-standard walls arising only when a mass-dependent fine tuning was imposed.

Furthermore, our primary motivation is the study of contact interactions (point interactions and reflecting walls) in phase-space quantum mechanics. So, it is the sharpness of the interactions that is most important to us, not their finiteness. We will therefore study here a non-sharp, or smoothed version of the Šeba potential, rather than of the potential in [38].

The authors of [38] speculate that a better choice than their piece-wise flat, discontinuous potential might eliminate the peculiar mass-dependent fine tuning required for non-standard walls. Presumably, it could also be argued to be possible for the

Šeba potential [68]. We will find, however, that the mass-dependent fine tuning remains necessary in a smoothed version of Šeba's potential. In retrospect, this should perhaps not be surprising, at least for Schrödinger quantum mechanics. The limit that squeezes and stretches the potentials into an infinite wall is so extreme, it seems unimportant whether the original potential has corners or is smoothed.

3.5 Wave functions with Robin boundary conditions from a Morse potential

To study how Robin boundary conditions arise in deformation quantization we will carry out an analysis similar to that of the previous section, but for a smooth potential. The spectrum is first found for a potential with undetermined parameters. Then we consider a certain limit of the parameters, demanding that we recover the infinite wall, and that the states recovered coincide with the eigenstates for the infinite wall, with Robin boundary conditions obeyed. For a smooth potential, it is guaranteed that the same potential that works for wave functions will also be suitable in deformation quantization.

The Šeba potential, with its sharp, zero-width features would cause the same kind of problem found when trying to quantize an infinite potential wall in phase space. Therefore it can only provide a guideline and we need to replace it with a similar smooth potential. A suitable candidate must depend continuously on a free parameter α as in (3.34), so that we recover the infinite potential wall in the $\alpha \to \infty$ limit. With its short range repulsion and longer range attraction, the smooth Morse potential is a rough approximation to Šeba's. Motivated by the shape resemblance it is natural to choose

$$V(q) \;=\; \frac{\hbar^2\kappa^2}{2m}\left(e^{-2\alpha q} - b\, e^{-\alpha q}\right) \;. \tag{3.45}$$

Besides α, two more parameters are needed – κ determines the overall potential strength, $b \geq 0$ the position of the well, and together they fix its depth. We will need to impose conditions on the coefficients in order to obtain Robin boundary conditions in the large α limit.

To provide insight into the possible behaviour of the coefficients in that limit, we compare the properties of the Šeba and Morse potentials. The latter has depth equal to $V_{\min} = V(q_{\min}) = -\hbar^2 b^2 \kappa^2 / 8m$ with $q_{\min} = -\ln(b/2)/\alpha$. The area between the curve and the q-axis can be found by integrating from its sole zero $q_0 = -\ln b/\alpha$ to infinity: $\hbar^2 \kappa^2 b^2 / 4m\alpha$. A comparison with the Šeba potential leads us to expect that $\kappa \sim \alpha$ and $b \sim \alpha^0$ (i.e. it is a dimensionless finite number), to leading order in α, for $\alpha \to \infty$.

The previous section indicates that we need only show that Robin boundary conditions apply at $q = \epsilon$, where epsilon is very small, but beyond the features of the Morse potential when $\alpha \to \infty$. For the unbound wave functions, therefore, we need only require that the relevant wave functions have the asymptotic form $\psi(q) \sim A \sin(kq + \phi)$ as $q \to \infty$, with ϕ variable.

To do that we first need to find the unbound wave functions. Following Matsumoto [59], we can solve the stationary Schrödinger equation for the Morse potential (3.45). The substitution $\psi(q) = \phi(z)$, $z = \exp(-\alpha q)$, changes the Schrödinger equation into

$$z^2 \phi'' + z\phi' + \frac{1}{\alpha^2} \left[\frac{2mE}{\hbar^2} - \kappa^2 z^2 + \kappa^2 b \, z \right] \phi = 0 \, . \tag{3.46}$$

This can be further transformed into canonical form (without a first derivative term) using the substitution $\phi(z) = z^{-1/2} F(z)$. Changing the variables to $y := 2\kappa z/\alpha$ leads to the so-called Whittaker equation, treated in [77], Chapter XVI:

$$f'' + \left\{ -\frac{1}{4} + \frac{b\kappa}{2\alpha} \frac{1}{y} + \frac{1}{y^2} \left[\frac{1}{4} - \left(\frac{ik}{\alpha} \right)^2 \right] \right\} f = 0 \, , \tag{3.47}$$

where $f(y) := F(\alpha y/2\kappa)$ and, as before, $k = \sqrt{2mE}/\hbar$. The two linearly independent solutions are defined in [62], p.755. They are called Whittaker functions and can be expressed in terms of the Tricomi confluent hypergeometric function $U(\mu, \nu, z)$ and the Kummer confluent hypergeometric function $M(\mu, \nu, z)$: [9]

$$M_{lm}(z) = z^{m+1/2} e^{-z/2} \, M(1/2 + m - l, 1 + 2m; z) \ , \tag{3.48}$$

$$W_{lm}(z) = z^{m+1/2} e^{-z/2} \, U(1/2 + m - l, 1 + 2m; z) \ . \tag{3.49}$$

For our purposes, we only need the definitions of those functions

$$M(\mu, \nu; z) = \sum_{n=0}^{\infty} \frac{(\mu)_n}{(\nu)_n} \frac{y^n}{n!} \ , \tag{3.50}$$

$$\begin{aligned} U(\mu, \nu; z) = {} & \frac{\Gamma(\nu - 1)}{\Gamma(\mu)} z^{1-\nu} M(1 + \mu - \nu, 2 - \nu; z) \\ & + \frac{\Gamma(1 - \nu)}{\Gamma(\mu - \nu + 1)} M(\mu, \nu; z) \ . \end{aligned} \tag{3.51}$$

Here we use the Pochhammer symbol $(\mu)_n := \mu(\mu + 1)...(\mu + n - 1), \ (\mu)_0 := 1$.

Now the wave function can be written as

$$\psi_k(q) = e^{\alpha q/2} \left[C_1 M_{\frac{b\kappa}{2\alpha}, \frac{ik}{\alpha}}(y(q)) + C_2 W_{\frac{b\kappa}{2\alpha}, \frac{ik}{\alpha}}(y(q)) \right] \ . \tag{3.52}$$

Demanding a real wave function yields $C_1 = 0$. The second term has real values and it has physical asymptotic behaviour: it becomes a free wave for large positive q. It has a sinusoidal behaviour with a phase that depends on the potential parameters. For negative q, far from the origin, there is the expected rapid exponential decay of

[9] The Whittaker function $M_{lm}(z)$ should not be confused with the Kummer function $M(\mu, \nu, z)$ in the above equation. Subscripts are used to denote the parameters of the Whittaker functions in the literature, and the explicit bracket notation is used for confluent hypergeometric functions. For further information involving the hypergeometric functions see [62], p.753 and [1], p.503-506.

a classically forbidden region. The wave function is therefore

$$\psi_k(q) = Ce^{\alpha q/2} W_{\frac{b\kappa}{2\alpha},\frac{ik}{\alpha}}\left(\frac{2\kappa}{\alpha}e^{-\alpha q}\right) \ . \tag{3.53}$$

With the help of equation (3.51) we can rewrite this result in a form similar to that given by Matsumoto in [59] for a Morse potential with $b = 2$. The wave function is manifestly real in this form:

$$\begin{aligned}\psi(y) \ &= \ Ce^{-y/2}\,\tilde{A}\,y^{ik/\alpha}\,M\left(\frac{1}{2}-\frac{b\kappa}{2\alpha}+\frac{ik}{\alpha},1+\frac{2ik}{\alpha};y\right)+ \\ &+ Ce^{-y/2}\,\tilde{A}^*\,y^{-ik/\alpha}\,M\left(\frac{1}{2}-\frac{b\kappa}{2\alpha}-\frac{ik}{\alpha},1-\frac{2ik}{\alpha};y\right) \ ,\end{aligned} \tag{3.54}$$

with $C^* = C$ a normalization constant. The constant $\tilde{A}$ is significant because it will determine the phase:

$$\tilde{A} = \frac{\Gamma(-\frac{2ik}{\alpha})}{\Gamma\left(\frac{1}{2}-\frac{b\kappa}{2\alpha}-\frac{ik}{\alpha}\right)} \ . \tag{3.55}$$

Let us now examine the asymptotic behaviour of the wave function and how it depends on the parameters. In the limit $\alpha \to \infty$, $\exp(-y/2) \sim \exp(-e^{-\alpha q})$ approaches the step function, so the dynamics will be restricted to the positive half-line. The limit $q \to \infty$ corresponds to $y \to 0$. Using (3.54) and (3.51) we obtain

$$\psi(q) \ \sim \ C|\tilde{A}|\,\cos\Big[k\,q - \arg(\tilde{A})\Big] \ . \tag{3.56}$$

The phase can be calculated from (3.55) and Euler's infinite product formula

$$\frac{1}{\Gamma(u)} \ = \ ue^{\gamma u}\prod_{n=1}^{\infty}\Big[\Big(1+\frac{u}{n}\Big)\,e^{-u/n}\Big] \ . \tag{3.57}$$

A short calculation shows that

$$\arg(\tilde{A}) = \frac{\pi}{2} + \frac{\gamma k}{\alpha} \; - \\ \sum_{n=0}^{\infty} \left\{ \frac{k}{\alpha(n+1)} \; - \; \tan^{-1}\left[\frac{2k}{\alpha(n+1)}\right] \; + \; \tan^{-1}\left[\frac{2k}{(2n+1)\alpha - b\kappa}\right] \right\} . \tag{3.58}$$

Apart from the $\pi/2$, all terms will vanish in the $\alpha \to \infty$ limit, except those of the form $\tan^{-1}\left[2k/\left((2n+1)\alpha - b\kappa\right)\right]$. For one such term to survive the limit, we need $\kappa = \mathcal{O}(\alpha^1)$, as expected from our earlier analysis. If the strength κ does not have this form, we will recover Dirichlet boundary conditions, i.e. the standard wall. Now, since it is $b\kappa$ that is relevant, we let b absorb the proportionality constant, and use $\kappa = \alpha + \mathcal{O}(\alpha^0)$. Finally, because the terms of order α^0 and lower will not affect the results, we drop them, and put $\kappa = \alpha$ from now on.

In order to realize Robin boundary conditions (3.28), the parameter b must be of the special form

$$b = \; (2n+1) - \; 2L^{-1}/\alpha \; + \; \mathcal{O}(\alpha^{-2}) \; . \tag{3.59}$$

Here L is a fixed length, independent of α. Then we find

$$kL = \tan \arg(\tilde{A}) \tag{3.60}$$

in the large α limit, so that the wave function (3.54) does indeed satisfy the Robin boundary conditions (3.28) in the limit $\alpha \to \infty$.

At large α the term $2L^{-1}/\alpha$ is negligible compared to the other two. While the parameter b approaches an odd integer the second infinitesimal term is crucial. Apparently we need to fine tune the parameter b to recover the Robin boundary conditions. A version of this phenomenon has already been encountered in [38] where the parameters can only take very limited values. The authors argue that fine tuning may be a result of the particular choice of potential they are using, possibly because

it is not smooth. Since our analysis, using a smooth potential, produces a version of fine tuning as well, fine tuning cannot be related to discontinuity alone.

Let us see how the other extreme case, i.e. Neumann boundary conditions, arise. Using (3.55) we get that for $\alpha \to \infty$

$$\arg(\tilde{A}) \sim \frac{\pi}{2} + \arg\left(\frac{1}{2} - \frac{b\kappa}{2\alpha} - \frac{ik}{\alpha}\right) + \sum_{n=1}^{\infty} \arg\left(1 + \frac{1/2 - b\kappa/2\alpha - ik/\alpha}{n}\right) . \tag{3.61}$$

Taking into account that $\arg(z)$ has a branch cut on the negative real axis and that the energy E is given (k is fixed) we can now take the limit $\alpha \to \infty$.

Since $\kappa = \alpha$, if we want non-standard walls to survive, the parameter $b = 0$ will give phase $\pi/2$ coming from the first term. For $b = 1$ there will be a contribution $-\pi/2$ from the second term so that the overall phase will vanish. The sum will start to contribute for $b > 1$ and for each $n < \frac{b-1}{2}$ we need to add $(b/2 - 1)\pi$ to the phase. In other words for all even integers we will get an integer multiple of π which can at most change the sign in the $\cos(k\,q + \text{phase})$ function plus a $\pi/2$ which will turn the $\cos(k\,q + \text{phase})$ into a $\sin(k\,q)$. Thus the boundary conditions will always be Dirichlet. For odd integers we use the same argument except we will pick up additional $\pi/2$ when $n = \frac{b-1}{2}$. In that case the wave function's asymptotics will be a cosine one, i.e. Neumann boundary conditions will arise.

Different limits result for different values of b because the width and the depth of the potential both depend on it. Generically, Dirichlet boundary conditions are realized. For non-standard walls, we must fine-tune the parameters so that we are near Neumann boundary conditions. Notice that this is precisely as it was for the Šeba potential of sect. 2 (see (3.43) and nearby). Put another way, the fine-tuning is again to a reflection resonance, or slightly off its peak.

Let us now consider the bound states and their behaviour at large α. Their wave

functions are given in [37] as

$$\psi(q) \propto \exp(-\kappa e^{-\alpha q}/\alpha) e^{-\alpha(\nu - b\kappa/2\alpha + 1/2)q} L_\nu^{b\kappa/\alpha - 2\nu - 1}(2\kappa e^{-\alpha q}/\alpha) \ , \tag{3.62}$$

where

$$L_n^\lambda(q) = \sum_{m=0}^{n} (-1)^m \binom{n+\lambda}{n-m} \frac{q^m}{m!} \tag{3.63}$$

are the associated Laguerre polynomials $L_n^\lambda(q)$. The energies are

$$E_\nu = -\frac{\hbar^2 \alpha^2}{2m} (\nu - b\kappa/2\alpha + 1/2)^2 \, , \tag{3.64}$$

for integer $\nu \in [0, \lfloor b\kappa/2\alpha \rfloor]$, where $\lfloor a \rfloor$ is the smallest integer less than a.

Consider now the $\alpha \to \infty$ limit. The Laguerre polynomials are normalized to one at zero argument, and $\exp(-\kappa e^{-\alpha x}/\alpha)$ turns into the step function. The only term that remains to be analyzed is $e^{-\alpha(\nu - b\kappa/2\alpha + 1/2)x}$. Clearly, $-\alpha(\nu - b\kappa/2\alpha + 1/2)$ must be a negative constant (independent of α) so that we have a normalizable wave function that does not disappear in the large α limit. Again we can set $\kappa = \alpha$, and the solving for b yields precisely equation (3.59). Analyzing the bound states provides an alternative way of deriving the fine tuning condition.

On the other hand, let us give particular values to the constants in (3.59), i.e. fix b. All the bound states will vanish for $x > 0$ except the one that has highest quantum number $\nu = \lfloor b/2 \rfloor$. This is because the maximal integer will cancel the integer part of b and leave only the fine tuning part $-2(L\alpha)^{-1}$. The bound state wave function $\sim e^{-q/L}$ will be recovered with the correct energy $-\hbar^2/2mL^2$.

To summarize, in this section we demonstrated that the $\alpha \to \infty$ limit of the Morse potential (3.45) can be used to generate Robin boundary conditions. Fine tuning is necessary, however: the parameter b must be an odd non-negative integer plus a term with asymptotics $1/\alpha$ that determines the length scale L of the Robin boundary

condition. If the fine tuning is absent or if the integer part of b is not an odd integer, then we can only recover Dirichlet boundary conditions, i.e. standard walls. A new observation is that the fine-tuning selects a reflection resonance.

Notice that the definition of κ involves the particle mass. So, if the particle mass changes, so must the potential. The fine tuning required is also mass dependent.

The situation is very similar to that for the discontinuous Šeba potential [68] treated in sect. 2, and to the results of [38]. The mass-dependent fine-tuning that is necessary for non-standard (Robin boundary condition) walls seems to be more than an artifact of the choice of potential. In particular, just smoothing out the discontinuities of a piece-wise flat potential is not sufficient to avoid this property. As already stated, this is perhaps reasonable in hindsight: it seems that the limit that squeezes and stretches the potentials into an infinite wall is so extreme that it is unimportant whether the original potential has corners or is smoothed.

3.6 Deformation quantization with a Morse potential

Let us recall the definition of Wigner functions and the Wigner-Weyl correspondence (see [79, 43], e.g.). The Wigner function is related to the density operator of canonical quantization. More generally, every operator $\hat{Q}$ has a Weyl *symbol* $Q(x,p)$ defined by

$$\begin{aligned} Q(q,p) \;&=\; \mathcal{W}\hat{Q} \;=\; \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} d\xi d\eta \;\mathrm{Tr}\left[\hat{Q}\, e^{-i(\xi\hat{q}+\eta\hat{p})}\right] e^{i\xi q+i\eta p} \\ &=\; \frac{1}{2\pi}\int_{-\infty}^{\infty} dy\; e^{-iyp}\;\langle q+\hbar y/2|\hat{Q}|q-\hbar y/2\rangle\;. \end{aligned} \tag{3.65}$$

the Wigner transform is a map $\mathcal{W}:\;\hat{Q}\mapsto Q(x,p)$, from operators to phase space functions/distributions. It is a homomorphic map from the algebra of operators to

the $*$-algebra of symbols:

$$\mathcal{W}(\,\hat{Q}\,\hat{R}\,) \;=\; \mathcal{W}(\hat{Q}) \,*\, \mathcal{W}(\hat{R})\;. \tag{3.66}$$

Here the symbols are multiplied using the Moyal $*$-product,

$$* \;=\; \exp\left\{\,\frac{i\hbar}{2}\,\left(\,\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q}\,\right)\,\right\} \tag{3.67}$$

for consistency with the Wigner transform (3.65). We will also use here the inverse map $\mathcal{W}^{-1}$, i.e. the Weyl map:

$$\hat{Q} \;=:\; \mathcal{W}^{-1}Q(x,p) = \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} d\xi\; d\eta\; dq\; dp\; Q(q,p)e^{i\xi(\hat{q}-q)+i\eta(\hat{p}-p)}\;. \tag{3.68}$$

In this section we turn our attention to the Wigner function. Recall that up to normalization, the Wigner function $\rho(x,p)$ is defined as the Wigner transform of the density operator $\hat{\rho}$:

$$\rho(q,p) \;:=\; \frac{1}{2\pi\hbar}\,\mathcal{W}\,(\,\hat{\rho}\,)\;\;, \tag{3.69}$$

and it describes the state of the system.

We consider the equation of motion for the Wigner function:

$$i\hbar\,\partial_t\rho(q,p,t) = [H,\rho(q,p,t)]_*\;, \tag{3.70}$$

where $[H,\rho]_* = H*\rho - \rho*H$. It can be expressed as a linear combination of stationary Wigner functions with time-dependent coefficients:

$$\rho(q,p,t) = \sum_{E_L,E_R} C_{E_LE_R}e^{-i(E_L-E_R)t/\hbar}\rho_{E_LE_R}(q,p)\;. \tag{3.71}$$

Here $\rho_{E_LE_R} = \mathcal{W}(|E_L\rangle\langle E_R|)/2\pi\hbar$ denotes the Wigner transform of a matrix element

of the density operator in the energy basis. As $*$-eigenfunctions, they can be found by solving the system of equations:

$$H * \rho_{E_L E_R}(q,p) = E_L \ \rho_{E_L E_R}(q,p) \ , \tag{3.72}$$

$$\rho_{E_L E_R}(q,p) * H = E_R \ \rho_{E_L E_R}(q,p) \ . \tag{3.73}$$

Alternatively, the Wigner transform

$$\rho_{E_L E_R}(q,p) = \int_{-\infty}^{\infty} dy \ e^{iyp} \ \langle q + \hbar y/2 | E_L \rangle \langle E_R | q - \hbar y/2 \rangle \tag{3.74}$$

allows them to be determined from the wave functions, if known. In the case of smooth potentials, the resulting Wigner functions are known to agree. Provided $\rho_{E_L E_R}$ are found using (3.72-3.73) we can indeed show that equation (3.70) is satisfied by (3.71).

For discontinuous potentials, however, that is not necessarily the case [29]. The example relevant here is the infinite wall, or equivalently, a particle confined to the half-line. AS we saw earlier, Dias and Prata [29] showed that the Wigner transform of the density operator only satisfies the $*$-eigenvalue equations if the free Hamiltonian is modified. No independent motivation was given for the change to the Hamiltonian, however. It was also assumed that the Wigner transform itself did not need to be adjusted.

An independent motivation was first suggested in [55]: self-adjointness of the Hamiltonian. The free Hamiltonian on the half-line is not self-adjoint. It does have self-adjoint extensions, however, and these correspond precisely to the possible boundary conditions (3.28) (see [11], e.g.). Subsequently, the self-adjointness of the Dias-Prata modified Hamiltonian was demonstrated in [31].

Here we are concerned with the assumption of an unmodified Wigner transform. That is, does the unmodified Wigner transform of the density operator provide the physical Wigner function? In [55], we answered in the affirmative, by treating the

infinite wall as the limit of a smooth, Liouville potential. Only the standard Dirichlet boundary conditions were recovered, however. Here we will show that non-standard walls can be realized in a similar way, using the Morse potential, and that the naïve Wigner transform does indeed work, for all Robin boundary conditions, describing both non-standard and standard walls.

The Wigner transforms of the density operator elements relevant to Robin boundary conditions have already been computed, in [75]. So, we need to solve the $*$-eigenvalue equations (3.72, 3.73) for the Morse Hamiltonian, take the limit $\alpha \to \infty$ as described in the last section, and compare.

The goal is therefore to perform "pure" deformation quantization by solving the $*$-eigenvalue equations directly, without reference to operators or wave functions. This will be done for the Morse potential considered in the previous section. We will use the Mellin transform to convert the $*$-eigenvalue equations to difference equations.

Let us first indicate that the Morse potential (3.45) with $b = 2$ has already been treated in [37]. The Wigner functions of the bound states were obtained from the known wave functions (3.62) using the integral transform (3.74). Equation (3.63) provides us with a way to evaluate the integral in closed terms using the modified Bessel functions $K_\nu(q)$. The substitutions $z = 2\exp(-\alpha q)$ and $w = \exp(-\alpha\hbar y/2)$ in (3.74) and the integral representation

$$K_\nu(z) = \frac{1}{2}\int_0^\infty dw\ w^{-(\nu+1)} e^{-\frac{1}{2}z(w+1/w)} \tag{3.75}$$

yields

$$\rho(z,p) \propto z^{2\nu-b+1} \sum_{l_1,l_2=0}^{\nu} \binom{b-\nu-1}{\nu-l_1} \binom{b-\nu-1}{\nu-l_2} \frac{(-z)^{l_1+l_2}}{l_1!\ l_2!}\ K_{l_1-l_2-2ip/\alpha}(z)\,. \tag{3.76}$$

We will use this idea later when dealing with Wigner transforms ourselves.

However, the authors of [37] do not obtain the bound-state Wigner functions by

solving their dynamical equations. We will do that here, and also find the unbound-state Wigner functions in the same way.

We'll use a new method that produces difference equations for potentials that are polynomials of an exponential in x.[10] This is important in its own right since solutions to the $*$-eigenvalue equations are difficult to find. Let us start with a more general Hamiltonian and then concentrate on the Morse potential in particular.

$$\begin{aligned} H(q,p) * \rho_{k_L k_R}(q,p) &= E_L\, \rho_{k_L k_R}(q,p) =: \frac{\hbar^2 k_L^2}{2m}\, \rho(q,p)\ , \\ \rho_{k_L k_R}(q,p) * H(q,p) &= E_R\, \rho_{k_L k_R}(q,p) =: \frac{\hbar^2 k_R^2}{2m}\, \rho(q,p)\ . \end{aligned} \tag{3.77}$$

These equations will be of infinite order in momentum-derivatives for a generic Hamiltonian of the form $p^2/2m + V(q)$:

$$\left(\frac{p^2 - \hbar^2 k_L^2}{2m}\right)\rho - \frac{\hbar^2}{8m}\partial_q^2\rho - \frac{i\hbar p}{2m}\partial_q\rho + \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\hbar}{2}\right)^n \partial_q^n V \partial_p^n \rho = 0\ , \tag{3.78}$$

$$\left(\frac{p^2 - \hbar^2 k_R^2}{2m}\right)\rho - \frac{\hbar^2}{8m}\partial_q^2\rho + \frac{i\hbar p}{2m}\partial_q\rho + \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\left(\frac{i\hbar}{2}\right)^n \partial_q^n V \partial_p^n \rho = 0\,. \tag{3.79}$$

However the exponential form of the Morse potential (3.45) allows them to be written as differential-difference equations since the exponentials will generate translations in the momentum. Their explicit form becomes

$$\begin{aligned} &\frac{\hbar^2}{8m}\partial_q^2\rho + \frac{i\hbar p}{2m}\,\partial_q\rho = \\ &\frac{\hbar^2\alpha^2}{2m}e^{-2\alpha q}\rho(q, p - i\hbar\alpha) - \frac{b\hbar^2\alpha^2}{2m}\,e^{-\alpha q}\rho\left(q, p - \frac{i\hbar\alpha}{2}\right) + \left(\frac{p^2 - \hbar^2 k_L^2}{2m}\right)\rho \end{aligned} \tag{3.80}$$

[10] Strictly speaking, a difference equation is obtained for any potential that is a linear combination of exponentials, $\exp(-\alpha_i q)$, $i = 1, \ldots, n$, say. That is not likely to be helpful, however, unless all the ratios α_i/α_j are rational.

and

$$\frac{\hbar^2}{8m}\partial_q^2\rho - \frac{i\hbar p}{2m}\partial_q\rho = \tag{3.81}$$
$$\frac{\hbar^2\alpha^2}{2m}e^{-2\alpha q}\rho(q,p+i\hbar\alpha) - \frac{b\hbar^2\alpha^2}{2m}\; e^{-\alpha q}\rho\left(q,p+\frac{i\hbar\alpha}{2}\right) + \left(\frac{p^2-\hbar^2k_R^2}{2m}\right)\rho\ .$$

The integral transform technique leads to further simplifications. Suppose the Wigner function can be written as

$$\rho(q,p) \;=\; R(u,p)\ , \quad u\ := 16e^{4\alpha q}\,. \tag{3.82}$$

The Mellin transform of the Wigner function is

$$W(s,p) \;:=\; \mathcal{M}\{R\}(s,p) \;=\; \int_0^\infty u^{s-1}\,R(u,p)\,du\ . \tag{3.83}$$

To transform (3.80) and (3.81) into difference equations for $W(s,p)$ we consider the inverse Mellin transform

$$R(u,p) \;=\; \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} u^{-s}\,W(s,p)\,ds\ , \tag{3.84}$$

where the constant c can be any constant for which the transform converges according to the Mellin inversion theorem.

3.6.1 Solution for the Liouville potential

We will first apply the method to the Liouville potential

$$V_L(q) \;=\; \frac{\hbar^2\kappa^2}{2m}\,e^{-2\alpha q}\ . \tag{3.85}$$

It is the simplest case as it can be viewed as a Morse potential for $b = 0$. Also, we can check our results since the Wigner functions for this potential have already been found in [24].

The $*$-eigenvalue equations (3.77) imply the difference equations

$$\begin{aligned}(p/\hbar + 2i\alpha s)^2 W_0(s,p) + (2\alpha)^2 W_0(s-1/2, p - i\alpha\hbar) &= k_L^2 W_0(s,p)\ , \\ (p/\hbar - 2i\alpha s)^2 W_0(s,p) + (2\alpha)^2 W_0(s-1/2, p + i\alpha\hbar) &= k_R^2 W_0(s,p)\ . \end{aligned} \tag{3.86}$$

Let us now assume that the solution is factorized into two parts – "left" and "right" factors – each depending on k_L or k_R only:

$$W(s,p) \;=\; N\, w_L\big(s - \frac{ip}{2\alpha\hbar},\, k_L\big)\, w_R\big(s + \frac{ip}{2\alpha\hbar},\, k_R\big)\ , \tag{3.87}$$

with N a normalization constant. For the left factor we find

$$\begin{aligned}(p/\hbar + 2i\alpha s)^2\, w_L(s - ip/2\alpha\hbar) + (2\alpha)^2\, w_L(s - ip/2\alpha\hbar - 1) = \\ = k_L^2\, w_L(s - ip/2\alpha\hbar)\end{aligned} \tag{3.88}$$

and for the right factor

$$\begin{aligned}(p/\hbar - 2i\alpha s)^2\, w_R(s + ip/2\alpha\hbar) + (2\alpha)^2\, w_R(s + ip/2\alpha\hbar - 1) = \\ = k_R^2\, w_R(s + ip/2\alpha\hbar)\ .\end{aligned} \tag{3.89}$$

Using the substitution $t = s - ip/2\alpha\hbar$ we arrive at

$$w(t-1, k_L) \;=\; \left[t^2 + \frac{k_L^2}{(2\alpha)^2}\right] w(t, k_L)\ . \tag{3.90}$$

Equation (3.89) also leads to the above equation if we use $t = s + ip/2\alpha\hbar$ and k_R

instead. Therefore we can only work with (3.88) and the solutions will differ only by a translation of the argument and the label of k.

The solution of (3.90) is

$$w(t, k_L) = \Gamma(-t + ik_L/2\alpha)\,\Gamma(-t - ik_L/2\alpha)\ , \tag{3.91}$$

by the defining property $\Gamma(z+1) = z\Gamma(z)$ of the gamma function. Tracing back to equations (3.87-3.88), (3.84) and (3.82), we can write the Wigner function in terms of the inverse Mellin transform:

$$\rho_{k_L k_R}(q,p) \propto \int_{c-i\infty}^{c+i\infty} ds \left(16 e^{4\alpha q}\right)^{-s} \times \prod_{\pm,\pm'} \Gamma\left(-s + \frac{i(p/\hbar \pm k_L)}{2\alpha}\right) \Gamma\left(-s - \frac{i(p/\hbar \pm' k_R)}{2\alpha}\right). \tag{3.92}$$

This last is an integral representation of the Meijer G-function. Using equation (43) on p.353 in [35] we can write the Wigner function as [11]

$$\rho_{k_L k_R}(q,p) \propto G^{40}_{04}\left(\frac{e^{-4\alpha q}}{16}\middle| \frac{i(p/\hbar + k_L)}{2\alpha}, \frac{i(p/\hbar - k_L)}{2\alpha}, -\frac{i(p/\hbar - k_L)}{2\alpha}, -\frac{i(p/\hbar + k_L)}{2\alpha}\right). \tag{3.93}$$

We also used the identity

$$G^{40}_{04}\left(u|1-a_1, 1-a_2, 1-a_3, 1-a_4\right) = G^{40}_{04}\left(1/u|a_1, a_2, a_3, a_4\right)\ . \tag{3.94}$$

As it should, the formula for the Wigner function (3.94) coincides with the one obtained using different methods in [24]. It describes the phase-space quasi-distribution for a particle in a Liouville potential. The advantage of the method proposed here is

[11] This result can also be found using supersymmetric quantum mechanics. In deformation quantization, the ladder operators are replaced by functions and a star product is used, however the transition is fairly straightforward [24].

that it can be generalized to the Morse potential.

3.6.2 Solution for the Morse potential

Now let us go back to the original problem of finding the Wigner function for the potential (3.45). Applying the same techniques we can treat any potential that is a polynomial in $\exp(-\alpha q)$. Therefore we can transform the differential equations of infinite order in p for the Morse potential into translations of the momentum and eventually into difference equations. The left $*$-eigenvalue equation has the form

$$\begin{aligned}(p/\hbar + 2i\alpha s)^2 W_b(s,p) + (2\alpha)^2 W_b(s-1/2, p-i\alpha\hbar) \\ -\frac{b}{2}(2\alpha)^2\, W_b(s-1/4, p-i\alpha\hbar/2) \;=\; k_L^2\, W_b(s,p)\;.\end{aligned} \tag{3.95}$$

We also have the complex conjugate (right) equation, with k_L replaced by $k_R = \sqrt{2mE_R}/\hbar$. To solve the new left difference equation (3.95), we substitute the ansatz (3.87) to obtain

$$\begin{aligned}(p/\hbar + 2i\alpha s)^2\, w_L(s - ip/2\alpha\hbar, k_L) + (2\alpha)^2\, w_L(s - ip/2\alpha\hbar - 1, k_L) \\ -\frac{b}{2}(2\alpha)^2\, w_L(s - ip/2\alpha\hbar - 1/2, k_L) \;=\; k_L^2\, w_L(s - ip/2\alpha\hbar, k_L)\;.\end{aligned} \tag{3.96}$$

Using the same substitution $t = s - ip/2\alpha\hbar$ as in (3.89) and switching to $w_b = w_L$ to account for the parameter dependence, we arrive at the difference equation for the Morse potential:

$$w_b(t-1, k_L) - \frac{b}{2}\, w_b(t-1/2, k_L) \;=\; \left[t^2 + \frac{k_L^2}{(2\alpha)^2}\right] w_b(t, k_L)\;. \tag{3.97}$$

This equation has a trivial solution for $b = 0$, since that is simply the Liouville case. The right factor satisfies an identical equation with k_L replaced by k_R and $t = s + ip/2\alpha\hbar$.

For $b = 1$ the solution can be written in terms of gamma functions, as in the $b = 0$ case

$$w_1(t,k) \propto \Gamma\left(-t + \frac{ik}{2\alpha}\right)\Gamma\left(-t + \frac{1}{2} - \frac{ik}{2\alpha}\right) + \Gamma\left(-t + \frac{1}{2} + \frac{ik}{2\alpha}\right)\Gamma\left(-t - \frac{ik}{2\alpha}\right). \tag{3.98}$$

The inverse Mellin transform then gives us the Wigner function:

$$\begin{aligned}\rho_{k_L k_R}(q,p) \propto & \\ & G^{40}_{04}\left(\frac{1}{u}\middle| \frac{ip}{2\alpha\hbar} + \frac{ik_L}{2\alpha}, \frac{1}{2} + \frac{ip}{2\alpha\hbar} - \frac{ik_L}{2\alpha}, -\frac{ip}{2\alpha\hbar} + \frac{ik_R}{2\alpha}, \frac{1}{2} - \frac{ip}{2\alpha\hbar} - \frac{ik_R}{2\alpha}\right) + \\ & G^{40}_{04}\left(\frac{1}{u}\middle| \frac{ip}{2\alpha\hbar} + \frac{ik_L}{2\alpha}, \frac{1}{2} + \frac{ip}{2\alpha\hbar} + \frac{ik_L}{2\alpha}, \frac{1}{2} - \frac{ip}{2\alpha\hbar} + \frac{ik_R}{2\alpha}, -\frac{ip}{2\alpha\hbar} - \frac{ik_R}{2\alpha}\right) + \\ & G^{40}_{04}\left(\frac{1}{u}\middle| \frac{1}{2} + \frac{ip}{2\alpha\hbar} + \frac{ik_L}{2\alpha}, \frac{ip}{2\alpha\hbar} - \frac{ik_L}{2\alpha}, -\frac{ip}{2\alpha\hbar} + \frac{ik_R}{2\alpha}, \frac{1}{2} - \frac{ip}{2\alpha\hbar} - \frac{ik_R}{2\alpha}\right) + \\ & G^{40}_{04}\left(\frac{1}{u}\middle| \frac{1}{2} + \frac{ip}{2\alpha\hbar} + \frac{ik_L}{2\alpha}, \frac{ip}{2\alpha\hbar} - \frac{ik_L}{2\alpha}, \frac{1}{2} - \frac{ip}{2\alpha\hbar} + \frac{ik_R}{2\alpha}, -\frac{ip}{2\alpha\hbar} - \frac{ik_R}{2\alpha}\right).\end{aligned} \tag{3.99}$$

This $b = 1$ Wigner function will correspond to Neumann boundary conditions in the $\alpha \to \infty$ limit, as we will show in the next section, in agreement with eqn. (3.59) and the arguments preceding it.

Another solution that is easy to find[12] is for $b = 2$:

$$w_2(t,k) \propto (t + 1/4)\prod_{\pm}\Gamma\left(-t \pm \frac{ik}{2\alpha}\right) - \prod_{\pm}\Gamma\left(-t + \frac{1}{2} \pm \frac{ik}{2\alpha}\right). \tag{3.100}$$

It can be written in a different form which shows a pattern shared with the case $b = 1$:

$$\begin{aligned}w_2(t,k) \propto & (2ik/\alpha + 1)\,\Gamma(-t + ik/2\alpha)\,\Gamma(-t + 1 - ik/2\alpha) + \\ & \frac{4ik}{\alpha}\,\Gamma(-t + 1/2 + ik/2\alpha)\,\Gamma(-t + 1/2 - ik/2\alpha) + \\ & (2ik/\alpha - 1)\,\Gamma(-t + 1 + ik/2\alpha)\,\Gamma(-t - ik/2\alpha).\end{aligned} \tag{3.101}$$

[12] This can also be confirmed using supersymmetric quantum mechanics.

The Wigner function can be found with a trivial but lengthy calculation that is essentially identical to the $b = 0$ and $b = 1$ cases. Since it recovers the Dirichlet boundary condition the exact combination of Meijer G-functions is not of interest to us.[13]

A useful observation is that the left factors (for different b) can be written as:

$$w_1 = C_1 w_0(t - 1/4, k + i\alpha/2) + C_2 w_0(t - 1/4, k - i\alpha/2) \tag{3.102}$$

and

$$w_2 = C_1 w_0(t - 1/2, k + i\alpha) + C_2 w_0(t - 1/2, k) + C_3 w_0(t - 1/2, k - i\alpha)\ . \tag{3.103}$$

A closer examination of the known solutions suggests that by choosing the constants correctly we can write the solution for any integer b:

$$w_b(t, k) \propto \sum_{n=-\frac{b}{2}, -\frac{b}{2}+1, \ldots, \frac{b}{2}} C_n^b \, w_0\left(t - b/4, k - in\alpha\right). \tag{3.104}$$

We can substitute this ansatz into the equation (3.97) using undetermined coefficients. In principle, comparison of the coefficients of independent terms can determine C_n^b for any b. This seems to fail, however, in the case of non-integer b. Furthermore, even for the simplest cases this program is very difficult to carry out. Clearly we need an algorithm that reproduces the constants directly and allows a generalization to include all Morse potentials of the form (3.45).

3.6.3 Systematic solution of the difference equations

In order for our method to be a fully-fledged pure deformation quantization treatment, we need an algorithm that reproduces the solutions for all values of b. We now present

[13] We will derive a general expression that includes this one later on.

such an algorithm and find the relevant solutions for the Morse potential. We exploit once again the property of the Mellin transform to relate differential equations and their solutions to difference equations and their solutions.

To convert our difference equation (3.97) into a differential equation we use the following two properties of the Mellin transform:

$$\mathcal{M}\{\tau^2 f''(\tau) + \tau f(\tau)\}(s) = s^2 \mathcal{M}\{f(\tau)\}(s)\,, \tag{3.105}$$

$$\mathcal{M}\{\tau^a f(\tau)\}(s) = \mathcal{M}\{f(\tau)\}(s+a)\,. \tag{3.106}$$

If we apply the inverse Mellin transform directly to (3.97), we end up with an equation that we cannot solve. This is because the Mellin transform converts argument translations into powers of the argument via (3.106). To eliminate fractional powers, we use the substitution $s = 2t$. The new equation for $\tilde{w}_b(s) = w(t(s))$

$$\tilde{w}_b(s-2) - \frac{b}{2}\tilde{w}_b(s-1) = \left[\left(\frac{s}{2}\right)^2 + \frac{k^2}{(2\alpha)^2}\right]\tilde{w}_b(s) \tag{3.107}$$

results in a simpler, integrable equation:

$$\tau^2 f''(\tau) + \tau f'(\tau) + \left[(k/\alpha)^2 - 4/\tau^2 + 2b/\tau\right] f(\tau)\,, \tag{3.108}$$

where $\tilde{w}(s) = \mathcal{M}\{f(\tau)\}(s)$. The solution $f(\tau)$ of this equation can be found if we make the substitution $f(\tau) = \tau^{-1/2} g(\tau)$ and then $u(z) = g(t(z))$, where $z = 1/\tau$. The new function $u(z)$ solves the Whittaker equation already encountered, so we skip the details. The solution is:

$$f(\tau) = C_1 \tau^{1/2} M_{\frac{b}{2},\frac{ik}{\alpha}}(4/\tau) + C_2 \tau^{1/2} W_{\frac{b}{2},\frac{ik}{\alpha}}(4/\tau)\ . \tag{3.109}$$

This is the general solution and it therefore depends on two arbitrary constants. We

know from the previous subsections, however, that we must set $C_1 = 0$ to obtain the physical states.[14]

Let us confirm that (3.109) indeed recovers (3.91, 3.98, 3.101) and (3.104). For $b \in \mathbb{N}$ we can write the Whittaker W-function in terms of the modified Bessel functions

$$W_{\frac{n}{2},\mu}(y) = \frac{y^{\frac{n+1}{2}}}{\sqrt{\pi}} \left(\frac{1-n}{2} + \mu\right)_n \times \\ \times \sum_{k=0}^{n} \frac{(-1)^{n+k}(2k-n+2\mu)(-n)_{n-k}}{\Gamma(n-k)(k-n+2\mu)_{n+1}} K_{-k+\frac{n}{2}-\mu}\left(\frac{y}{2}\right) \ . \tag{3.110}$$

With the help of the integral representation of the Bessel functions (effectively finding the inverse Mellin transform),

$$K_\nu(z) = \frac{1}{4\pi i} \int_{c-i\infty}^{c+i\infty} \Gamma(s)\Gamma(s-\nu) \left(\frac{z}{2}\right)^{\nu-2s} ds \ , \tag{3.111}$$

we can find the solution of (3.107) for integer b:

$$w_b(t,k) \propto \sum_{n=0}^{b} \tilde{C}_n^b \, \Gamma\left(-t + n/2 + ik/2\alpha\right) \Gamma\left(-t - n/2 + b/2 - ik/2\alpha\right). \tag{3.112}$$

This is nothing more than (3.104) with a shifted summation index. The coefficients are now explicit, however:

$$\tilde{C}_n^b = \frac{(-1)^n(2n-b+2ik/\alpha)(-b)_{b-n}}{(b-n)!(n-b+2ik/\alpha)_{b+1}} \ . \tag{3.113}$$

The Wigner function can be found the same way as in the preceding two subsections, with result

$$\rho_{k_L k_R}(q,p) = \sum_{m,n=0}^{b} \tilde{C}_m^b \tilde{C}_n^b \times \tag{3.114}$$

[14] That is, after the relevant integral transformations; this solution itself does not have a direct physical meaning.

$$\times G_{04}^{40}\left(\frac{z^4}{16}\middle|\begin{matrix}\frac{n}{2}+\frac{i(p/\hbar+k_L)}{2\alpha},\frac{b}{2}-\frac{n}{2}+\frac{i(p/\hbar-k_L)}{2\alpha},\\ \frac{m}{2}-\frac{i(p/\hbar-k_R)}{2\alpha},\frac{b}{2}-\frac{m}{2}-\frac{i(p/\hbar+k_R)}{2\alpha}\end{matrix}\right).$$

Bound states can also be treated this way; one only needs to consider imaginary k, for energies $E<0$. The resulting form of the Wigner functions appears to differ from (3.76), however. To reconcile the two results, recall that the energies are given by (3.64) and we can write

$$f(\tau)\propto\tau^{1/2}W_{\frac{b}{2},\frac{ik}{\alpha}}(4/\tau)=\tau^{1/2}W_{\frac{b}{2},\frac{b}{2}-\nu-\frac{1}{2}}(4/\tau)\,. \tag{3.115}$$

The relationship

$$W_{a,a-\nu-\frac{1}{2}}(z)\;=\;(-1)^\nu\nu!\,z^{a-\nu}e^{-z/2}L_\nu^{2a-2\nu-1} \tag{3.116}$$

(for integer ν) and (3.63) allow us to write the solution as

$$f(\tau)\propto e^{-2/\tau}\sum_{l=0}^{\nu}\frac{(-1)^l}{l!}\binom{b-\nu-1}{\nu-l}\left(\frac{4}{\tau}\right)^{l+b/2-\nu-1/2}. \tag{3.117}$$

Transforming the above we find the corresponding factor:

$$w(t)\propto\sum_{l=0}^{\nu}\frac{(-2)^l2^{2t}}{l!}\binom{b-\nu-1}{\nu-l}\Gamma\left(-2t+l+b/2-\nu-1/2\right). \tag{3.118}$$

With the help of the inverse Mellin transform we recover (3.76) the same way as in the unbound case, using (3.111) and (3.84).

Now that we have confirmed that our results agree with those previously obtained, let us proceed to the case of non-integer b. For $b\in\mathbb{R}$, we will reap the full benefits of our method, by finding an explicit and closed expression for the solution of the difference equation. We start by rewriting the solution of the differential equation

(3.108) in terms of hypergeometric functions:

$$f(\tau) = e^{-2/\tau}\tau^{-ik/\alpha}U\left(\frac{1}{2} - \frac{b}{2} + \frac{ik}{\alpha}, 1 + \frac{2ik}{\alpha}; \frac{4}{\tau}\right) \ . \tag{3.119}$$

This is necessary in order to perform the inverse Mellin transform of $f(\tau)$ in closed terms, which presents a technical problem if we use the Whittaker function.

We use the relationship (3.51) between the Kummer and Tricomi hypergeometric function and the integral expression

$$e^{-\sigma x}M(\beta,\gamma;\lambda x) = \int_{c-i\infty}^{c+i\infty} ds\ x^{-s}\sigma^{-s}\,\Gamma(s)\ {}_2F_1(\beta, s\,;\gamma\,;\lambda\sigma^{-1}) \tag{3.120}$$

to make it possible to find the inverse Mellin transform of (3.119). It is given in term of the Gauss hypergeometric function ${}_2F_1$. Switching back to our original variable t we find

$$\begin{aligned} w_b(t) \propto\ & \frac{4^{t+ik/2\alpha}\Gamma(-2ik/\alpha)}{\Gamma(1/2-b/2-ik/\alpha)}\Gamma(-2t+ik/\alpha)\times \\ & {}_2F_1\left(1/2-b/2+ik/\alpha, -2t+ik/\alpha; 1+2\,ik/\alpha; 2\right) + \\ & \frac{4^{t-ik/2\alpha}\Gamma(2ik/\alpha)}{\Gamma(1/2-b/2+ik/\alpha)}\Gamma(-2t-ik/\alpha)\times \\ & {}_2F_1\left(1/2-b/2-ik/\alpha, -2t-ik/\alpha; 1-2\,ik/\alpha; 2\right) . \end{aligned} \tag{3.121}$$

This is the solution of the difference equation (3.97) for any $b \in \mathbb{R}$ including the ones we already found earlier.

Let us point out that, while of secondary interest to the problem of Robin boundary conditions, the method used here allows us to produce exact solutions of the $*$-eigenvalue equations for a family of potentials. In deformation quantization, this is important because exact solutions are not easy to find; non-local pseudo-differential equations are difficult to solve directly. The corresponding difference equations are less difficult and they allow systematic treatment. After factoring and then performing

an inverse Mellin transform, the problem of solving a pseudo-differential equation[15] boils down to solving an ordinary differential equation. It is likely that this technique can work for other potentials.

3.7 Wigner functions for Robin boundary conditions from a Morse potential

The Wigner function for unbound states in the Morse potential can now be written. Below we will verify that for $q > 0$, its $\alpha \to \infty$ limit produces the expected result [75], the Wigner transform of the density operator built from the wave functions (3.29, 3.30):

$$\rho(q,p) \propto \frac{\sin\left[2(p/\hbar - k)q\right]}{(p/\hbar - k)} + \frac{\sin\left[2(p/\hbar + k)q\right]}{(p/\hbar + k)} + 2\cos(2kq - \delta_k)\frac{\sin\frac{2}{\hbar}p\,q}{p/\hbar}\ . \quad (3.122)$$

Recall that for the Morse potential the Wigner function can be written in contour integral form (3.82, 3.84) using the inverse Mellin transform. By (3.87) the kernel of the transform is a product of left and right functions, so that

$$\rho_{k_L k_R}(q,p) \propto \int_{c-i\infty}^{c+i\infty} ds\, \left(16e^{4\alpha q}\right)^{-s} w_L(s,k_L)\, w_R(s,k_R)\ . \quad (3.123)$$

From (3.122), the left factor can be written as

$$\begin{aligned} w_L(t,k_L) \propto\ & \tilde{A}\Gamma\Big(-t + i(p/\hbar + k_L)/2\alpha\Big)\,\Gamma\Big(-t + i(p/\hbar + k_L)/2\alpha + 1/2\Big) \times \\ & {}_2F_1\Big(1/2 - b/2 + ik_L/\alpha, -2t + i(p/\hbar + k_L)/\alpha; 1 + 2\,ik_L/\alpha; 2\Big) + \\ & \tilde{A}^*\,\Gamma\Big(-t + i(p/\hbar - k_L)/2\alpha\Big)\,\Gamma\Big(-t + i(p/\hbar - k_L)/2\alpha + 1/2\Big) \times \\ & {}_2F_1\Big(1/2 - b/2 - ik_L/\alpha\hbar, -2t + i(p/\hbar - k_L)/\alpha\hbar; 1 - 2\,ik_L/\alpha; 2\Big)\ . \end{aligned} \quad (3.124)$$

[15] Equivalently, we find an integro-differential equation, if we use the integral representation of the $*$-product.

Here we have defined $A = 4^{ik/\alpha}\tilde{A}$, with $\tilde{A}$ as in (3.55), and used the identity $\Gamma(2z) \propto 2^{2z-1}\Gamma(z)\Gamma(z+1/2)$. Similarly, the right factor is found to be

$$\begin{aligned} w_R(t,k_R) \propto \tilde{A}\,\Gamma\Big(-t - i(p/\hbar - k_R)/2\alpha\Big)\,\Gamma\Big(-t - i(p/\hbar - k_R)/2\alpha + 1/2\Big) \times \\ {}_2F_1\Big(1/2 - b/2 + ik_R/\alpha, -2t - i(p/\hbar - k_R)/\alpha; 1 + 2\,ik_R/\alpha; 2\Big) + \\ \tilde{A}^*\,\Gamma\Big(-t - i(p/\hbar + k_R)/2\alpha\Big)\,\Gamma\Big(-t - i(p/\hbar + k_R)/2\alpha + 1/2\Big) \times \\ {}_2F_1\Big(1/2 - b/2 - ik_R/\alpha, -2t - i(p/\hbar + k_R)/\alpha; 1 - 2\,ik_R/\alpha; 2\Big)\,. \end{aligned} \tag{3.125}$$

Equations (3.123-3.125) display our general solution of the $*$-eigenvalue equations of phase-space quantum mechanics, for unbound states in a Morse potential (3.45) with arbitrary parameter $b \in \mathbb{R}$.

Following [55], we use the residue theorem to find the limit of the Wigner function when $\alpha \to \infty$. Since the calculation is straightforward but lengthy, we omit the details. The expression under the integral (3.122) has 4 terms, one proportional to $\tilde{A}^2$, one to $\tilde{A}^{*2}$ and two to $|\tilde{A}|^2$. The $|\tilde{A}|^2$-terms yield contributions proportional to $[\,e^{2iq(p/\hbar - k)} - e^{-2iq(p/\hbar - k)}]/(p/\hbar - k)$ and $[\,e^{2iq(p/\hbar + k)} - e^{-2iq(p/\hbar + k)}]/(p/\hbar + k)$. The $\tilde{A}^2$-term and the $\tilde{A}^{*2}$-term yield

$$\hbar[\,e^{2i\arg\tilde{A} + 2iqp/\hbar - 2iqk} - e^{2i\arg\tilde{A} - 2iqp/\hbar - 2iqk}]/p$$

and

$$\hbar[\,e^{-2i\arg\tilde{A} + 2iqp/\hbar + 2iqk} - e^{-2i\arg\tilde{A} - 2iqp/\hbar + 2iqk}]/p.$$

Note that all the terms arising from residues at $i(\pm p/\hbar \pm' k)/2\alpha + 1/2$ produce decaying exponential factors and therefore do not contribute. Also, the Gauss hypergeometric function ${}_2F_1(a,b;c;z)$ is analytic with respect to its second argument and $\tilde{\infty}$ is its only singularity. The contributions from ${}_2F_1(a,b;c;z)$ will manifest themselves as a

multiplication by constants in all cases. In particular, for those terms that survive in the limit of interest, the constant is 1.

The algebra can now be completed to reproduce the Wigner function for an infinite, but possibly non-standard wall (3.122) as we hoped. The Robin boundary conditions are indeed recovered using the Morse potential. We have outlined how the calculation is done for diagonal elements of the symbol of the density operator, but the non-diagonal case works in similar fashion.

As a check on our results, we'll now derive the Wigner functions for the unbound states using the Wigner transform. We will simplify equation (3.53) so that it is possible to perform the integral of (3.123) in closed terms. To do this we use (3.110) again, so that we must restrict consideration to $b \in \mathbb{N}$. The wave function, therefore, can be written in terms of $u = 2e^{-\alpha q}$ as

$$\psi(q) \;=\; N\, e^{-\alpha b q/2} \sum_{n=0}^{b} \tilde{C}_n^b \, K_{-n+b/2-ik/\alpha}(u(q)/2)\,, \tag{3.126}$$

with normalization constant

$$N \;=\; C(-1)^b 2^{(b+1)/2} \pi^{-1/2} (1/2 - b/2 + ik/\alpha)_b\ , \tag{3.127}$$

where C is the same constant as in (3.53), and the coefficients $\tilde{C}_n^b$ are given by (3.113). Using the substitution $w = e^{\alpha\hbar y/2}$, $z = e^{-\alpha q}$, we can rewrite (3.123) in terms of wave functions:

$$\rho_{k_L k_R} \propto z^b \sum_{m,n} \tilde{C}_m^b \tilde{C}_n^b \int_0^\infty dw\ w^{-2ip/\alpha\hbar - 1} K_{-n+\frac{b}{2}-\frac{ik_L}{\alpha}}\left(\frac{z}{w}\right) K_{-n+\frac{b}{2}-\frac{ik_R}{\alpha}}\left(zw\right)\ . \tag{3.128}$$

The last integral can be evaluated with the help of (25) in [35], vol. 2, pg. 375:

$$\int_0^\infty dw\ w^{\lambda-1} K_\mu\left(aw\right) K_\nu\left(\frac{b}{w}\right) = \tag{3.129}$$

$$\frac{2^{\lambda-3}}{a^\lambda} G_{04}^{40}\left(\frac{\alpha^2 b^2}{16}\middle|\, \frac{\nu}{2}, -\frac{\nu}{2}, \frac{\lambda+\mu}{2}, \frac{\lambda-\mu}{2}\right).$$

After a long but straightforward calculation we arrive at the final result

$$\rho_{k_L k_R}(q,p) = \sum_{m,n=0}^{b} \tilde{C}_m^b \tilde{C}_n^b \times$$
$$\times G_{04}^{40}\left(\frac{z^4}{16}\middle|\, \frac{n}{2} + \frac{i(p/\hbar + k_L)}{2\alpha}, \frac{b}{2} - \frac{n}{2} + \frac{i(p/\hbar - k_L)}{2\alpha},\right.$$
$$\left. \frac{m}{2} - \frac{i(p/\hbar - k_R)}{2\alpha}, \frac{b}{2} - \frac{m}{2} - \frac{i(p/\hbar + k_R)}{2\alpha}\right).$$

the Wigner function is a linear combination of Meijer G-functions, as expected. We can easily see that, at least for $b \in \mathbb{N}$, we recover the solutions from the previous section.

To find the Wigner function for real $b \notin \mathbb{N}$ is not so trivial. We were unable to perform the integral of the Wigner transform when it is expressed in terms of Whittaker or Kummer functions. It is possible to expand the integrand, however, and then integrate to derive an infinite-sum expression for the Wigner function. Using the substitutions $w = e^{-\alpha\hbar y/2}$ and $u = 2e^{-\alpha q}$, we can write

$$\rho(q,p) \propto \int_0^\infty dw\, w^{2ip/\alpha - 1} e^{-\frac{1}{2}u(w+1/w)} \times \tag{3.130}$$
$$\times \big[\tilde{A}^2\, u^{2ik/\alpha} M(\chi,\varsigma,u/w) M(\chi,\varsigma,zw) +$$
$$|\tilde{A}|^2\, w^{-2ik/\alpha} M(\chi,\varsigma,u/w) M(\bar{\chi},\bar{\varsigma},uw) +$$
$$|\tilde{A}|^2\, w^{2ik/\alpha} M(\bar{\chi},\bar{\varsigma},u/w) M(\chi,\varsigma,uw) +$$
$$(\tilde{A}^*)^2\, u^{-2ik/\alpha} M(\bar{\chi},\bar{\varsigma},u/w) M(\bar{\chi},\bar{\varsigma},uw)\big]\ .$$

Here $\chi := 1/2 - b/2 + ik/\alpha$ and $\varsigma := 1 + 2ik/\alpha$, and $\bar{\chi}$, $\bar{\varsigma}$, $\tilde{A}^*$ are the complex conjugates of χ, ς, $\tilde{A}$. Now using the definition (3.51) of the Kummer function, and the integral

expression

$$K_\nu(z) = \frac{1}{2}\int_0^\infty dw\ w^{-(\nu+1)} e^{-\frac{1}{2}z(w+1/w)}\,, \tag{3.131}$$

we obtain

$$\begin{aligned}\rho(q,p) \propto \sum_{m,n=0}^{\infty} \frac{u^{m+n}}{m!n!}\Bigg[\ & \tilde{A}^2 u^{2ik/\alpha}\frac{(\chi)_m(\chi)_n}{(\varsigma)_m(\varsigma)_n}K_{n-m-2ip/\hbar\alpha}(u) + \\ & |\tilde{A}|^2\frac{(\chi)_m(\bar{\chi})_n}{(\varsigma)_m(\bar{\varsigma})_n}K_{m-n+2i(k-p/\hbar)/\alpha}(u) + \\ & |\tilde{A}|^2\frac{(\bar{\chi})_m(\chi)_n}{(\bar{\varsigma})_m(\varsigma)_n}K_{m-n-2i(k+p/\hbar)/\alpha}(u) + \\ & (\tilde{A}^*)^2 u^{-2ik/\alpha}\frac{(\bar{\chi})_m(\bar{\chi})_n}{(\bar{\varsigma})_m(\bar{\varsigma})_n}K_{n-m-2ip/\hbar\alpha}(u)\Bigg]\ .\end{aligned} \tag{3.132}$$

The form of the Wigner function just obtained should be compared with eqns. (3.123-3.125) above. Let us sketch how to show the two expressions agree. After substituting (3.124) and (3.125) into (3.123), use the integral representation (3.111) of the Bessel functions to perform the integral over s. Then the definition

$${}_2F_1(a,b;c;z) \ = \ \sum_{n=0}^{\infty}\frac{(a)_n\,(b)_n}{(c)_n}\,\frac{z^n}{n!} \tag{3.133}$$

of the Gauss hypergeometric function recovers the result we get using the Wigner transform (3.132).

As a check, we will show now that the expression (3.132) just derived also reduces to (3.122) in the $\alpha \to \infty$ limit, as does (3.123-3.125). Let us focus on different terms in the sum of (3.132). Combining the first and last summands we get

$$\begin{aligned}&\left[\tilde{A}^2 e^{-2ikq}\frac{(\chi)_m(\chi)_n}{(\varsigma)_m(\varsigma)_n} + \tilde{A}^{*2}e^{2ikq}\frac{(\bar{\chi})_m(\bar{\chi})_n}{(\bar{\varsigma})_m(\bar{\varsigma})_n}\right]K_{n-m-2ip/\hbar\alpha}(z) \ = \\ &\quad\left|\frac{(\chi)_m(\chi)_n}{(\varsigma)_m(\varsigma)_n}\right|\cos\left(2kq - \arg\frac{\tilde{A}^2(\bar{\chi})_m(\bar{\chi})_n}{(\bar{\varsigma})_m(\bar{\varsigma})_n}\right)K_{n-m-2ip/\hbar\alpha}(z)\ .\end{aligned} \tag{3.134}$$

To determine the behaviour of the Wigner function for $z \sim 0$, we use the asymptotic

expansion of the modified Bessel functions

$$2K_\nu(z) \sim \Gamma(-\nu)(z/2)^\nu + \Gamma(\nu)(z/2)^{-\nu} \ , \tag{3.135}$$

and take the limit $\alpha \to \infty$. Only the zeroth order terms in (3.134) will survive

$$\begin{aligned} |\tilde{A}|^2 \left|\Gamma\left(-\frac{2ip}{\alpha\hbar}\right)\right| e^{i\arg\Gamma\left(-\frac{2ip}{\alpha\hbar}\right)} e^{2ipq/\hbar} \cos\left(2kq - 2\arg\tilde{A}\right) + \\ |\tilde{A}|^2 \left|\Gamma\left(\frac{2ip}{\alpha\hbar}\right)\right| e^{i\arg\Gamma\left(\frac{2ip}{\alpha\hbar}\right)} e^{-2ipq/\hbar} \cos\left(2kq - 2\arg\tilde{A}\right) \to \\ 2|\tilde{A}|^2 \cos\left(2kq - 2\arg\tilde{A}\right) \frac{\sin(2p\,q/\hbar)}{p/\hbar}, \end{aligned} \tag{3.136}$$

up to a normalization constant depending on α and $\hbar$. A similar calculation shows that the second and third terms of (3.132) can be combined and in the limit $\alpha \to \infty$ they become

$$|\tilde{A}|^2 \left[\frac{\sin\left(2q(p/\hbar - k)\right)}{p/\hbar - k} + \frac{\sin\left(2q(p/\hbar + k)\right)}{p/\hbar + k}\right] \ . \tag{3.137}$$

Putting (3.137, 3.136) together we obtain (3.122), with $\delta_k = 2\arg(\tilde{A})$, as shown already. We conclude that the Robin boundary conditions are recovered for all $b \in \mathbb{R}$.

3.8 Conclusion to contact interactions

In this chapter we concluded the treatment of infinite walls in phase space quantum mechanics by including the non-standard ones. Those were realized as limits of smooth potentials. It provides an alternative to the Dias-Prata and $*$-eigen-$*$ equation. Some of the results are independent of the formulation and are applicable in operator quantum mechanics.

Let us summarize our results. They are of two types: those untied to phase-space quantum mechanics, and those directly related to it. That is, some results involve

wave functions only, and others pertain to Wigner functions. We will list and discuss them in turn.

Wave functions

In section 4, we repeated Šeba's analysis [68] and showed that Robin boundary conditions (for wave functions) could be realized by a limit ($\alpha \to \infty$) of a discontinuous, piece-wise flat potential, eqn. (3.34). We pointed out that standard walls (Dirichlet boundary conditions) are generically realized in the limit, and non-standard walls arise only if a mass-dependent fine-tuning (3.38) is imposed; these observations are in agreement with those made in [38], for the limit of a similar, but everywhere finite, potential. The independent derivation of the fine-tuning condition from a study of the bound states, instead of just the continuum, is perhaps new. Also, we point out that the parameters are fine-tuned to a reflection resonance in the limit. If the fine-tuning is imposed, then non-standard walls can be realized, and the Robin length scale L is determined by exactly how the limit resonance is approached (see eqn. (3.43)).

The analysis of the piece-wise flat Šeba potential was repeated with a qualitatively similar, but smooth potential, the Morse potential of eqn. (3.45). Remarkably, the results were almost unchanged. Analysis of both the unbound and bound states yielded a mass-dependent fine tuning (3.59) required for non-standard boundary conditions. Again, a reflection resonance is selected by the fine tuning, and how the resonance is approached in the $\alpha \to \infty$ limit determines the precise boundary conditions realized, i.e., the Robin length scale L.

The results for the piece-wise flat Šeba potential and the smooth Morse potential are likely so similar because the limit required to obtain Robin boundary conditions is quite severe. The potential must be pinched and stretched to such extremes that it is not important whether the potential is smooth or has corners.

Let us comment on the fine tuning phenomenon. As mentioned in the introduction, the infinite reflecting wall is perhaps the simplest example of a so-called contact interaction. For such, the interaction imposes boundary or matching conditions, such as the Robin boundary conditions on the half line. Alternatively, the same conditions can be found by demanding that the Hamiltonian or its extension be self-adjoint (see [11]).

It has been emphasized that the non-standard versions of such interactions should not be ignored, since they may describe interesting physics [14, 38]. However, considerations of symmetry (such as time-reversal invariance, e.g.) can eliminate possibilities in some cases [23]. Can the physical possibilities be restricted in other ways?

Here we have assumed that contact interactions can only be realized physically as limits of smoother, less localized interactions. In agreement with the results of others [68, 38], mass-dependent fine tuning was found to be necessary for non-standard walls to emerge. We believe that this fine tuning explains why standard quantum walls, with their Dirichlet boundary conditions, are standard. Non-standard walls are unlikely to be realized physically, because the required fine tuning is improbable.[16]

It would be interesting to see if the realizations of other contact interactions as limits require similar fine tuning, and if there are so-called standard boundary/matching conditions selected that way.

Wigner functions

Our primary motivation came from phase-space quantum mechanics, or deformation quantization. In that context, we made some progress on solving the dynamical equations of Wigner functions. We pointed out that the Mellin transform can convert the $*$-eigenvalue equations (3.77-3.79) into simpler difference equations, if the

[16] This is reminiscent of the result of [13], where the renormalization of a different singular interaction was shown to select a preferred self-adjoint extension.

potential is polynomial in an exponential. Exploiting this method, we found easily the known [24] stationary Wigner functions (3.93, 3.94) for the Liouville potential.

The $*$-eigenvalue equations for the Morse potential, eqns. (3.80, 3.81), were then studied. Their Mellin transform yields difference equations, eqn. (3.95) and its complex conjugate. Factorization was then assumed, and a simple difference equation (3.97) with parameter b resulted. The Liouville solution works for $b = 0$, and new solutions were found directly for $b = 1$ and $b = 2$. They led to a general ansatz, eqn. (3.104), that would be verified later.

To find general solutions, after the Mellin transform and factorization, the inverse Mellin transform was applied, to obtain a solvable differential equation, (3.108). For $b \in \mathbb{Z}$, a solution (3.114, 3.113) to the $*$-eigenvalue equation was found. The more general solution, valid for all $b \in \mathbb{R}$, was written in 3.123, 3.124, 3.125).

Our solutions of the Morse $*$-eigenvalue equations were confirmed by calculating the Wigner transform of the density operator using the known wave functions.

Finally, we were able to demonstrate that in the sharp limit, our Wigner functions become those constructed by the Wigner transform from wave functions with Robin boundary conditions. Specifically, we showed that when $\alpha \to \infty$, equations (3.123, 3.124, 3.125) reduce to the expected Wigner function, eqn. (3.122) [75], $x > 0$. This justifies the assumption that the Wigner transform is unmodified for these examples of contact interactions.

Chapter 4

Dissipative quantum mechanics via deformation quantization

In this chapter we study dissipative phenomena in terms of phase space distributions and star products in the framework of deformation quantization. We first present a short review of some relevant well-known techniques. We then develop a treatment of damped harmonic oscillator based on a modified star product originally proposed in [32] a few years ago. It is our belief that deformation quantization is a natural language for the treatment of dissipative systems and its applications to the subject should be further investigated. Used by itself or together with the standard operator and path integral treatments it can provide a better understanding of dissipative physics.

4.1 Introduction

The quantum mechanics of dissipative systems has been studied intensively; for reviews, see [28, 66, 76]. Work started soon after the birth of quantum mechanics and continues today. There are various methods developed to treat dissipative systems. Perhaps the most fundamental approach is to consider the system of interest as in-

teracting with an appropriate reservoir. Then the well-known quantization methods that are valid for non-dissipative, closed systems can be applied to the system plus reservoir as a whole. Effective equations of motion for the system can then be found by integrating out the reservoir degrees of freedom, while making appropriate physical assumptions. We will present the Caldeira-Leggett treatment as an example. Conceptually clear and physically compelling as this program is, it presents us with a problem known from statistical physics. As the size of the reservoir increases, so does the complexity of the mathematical description. Clearly for particular problems it would be beneficial to have effective approaches that allow us to extract the correct physics as an approximation to the program proposed earlier.

The effective approach technique is to work backwards, and derive the effective equations by adapting quantization procedures to non-dissipative systems. The adapted quantization procedures should, in the end, agree with more fundamental treatments. Provided they do, they would be helpful, as shortcuts for the more fundamental derivations, and possibly more. Curiously enough the methods used are remarkably inhomogeneous, in both ideas and mathematical description, compared to their non-dissipative counterparts. The effective treatment of such systems is more difficult, both classically and quantum mechanically. Overall we tend to stick to ideas that are proven to be effective, like the Hamiltonian formalism. However we have to give up certain features of the formalism to accommodate dissipation. The question is then which features of the non-dissipative physics are physically important and which are not and what will replace the latter.

This chapter is organized as follows. The first section will provide a brief but hopefully self-contained summary of some of the approaches to quantization of dissipative systems. Canonical (operator) quantization has been adapted to dissipative systems either by using time-dependent Hamiltonians, complex Hamiltonians, or by modifying the canonical Poisson brackets, and the corresponding operator commuta-

tors.[1] Dekker's complex Hamiltonian, Caldeira-Leggett, Bateman's Hamiltonian and the Lindblad equation are some of the treatments we will discuss. We will compare those with the deformation quantization method discussed in the second part. Of course we will leave out an enormous amount of information since it is impossible to fit it in an introductory chapter. However we have observed certain properties arising from the deformation treatment that point to possible relationships with the above.

As already mentioned, in the second section we concern ourselves with a different quantization method: quantum mechanics in phase space, or deformation quantization. Specifically, we study Dito and Turrubiates' [32] recent adaptation of deformation quantization to the paradigmatic dissipative system, the damped harmonic oscillator. The important innovation they introduce is a non-Hermitian γ-deformation of the Moyal star product of non-dissipative deformation quantization, where γ denotes the damping constant. Their damped star product is built in turn on a γ-deformation of the classical Poisson bracket, and so recalls the modified brackets of canonical operator quantum mechanics adapted to dissipation that were just mentioned. Perhaps this is not surprising, since canonical classical mechanics is a key ingredient of deformation quantization; the algebra of quantum observables is described as an $\hbar$-deformation of the classical Poisson algebra on phase space. Unlike in other schemes, the one proposed by Dito and Turrubiates *only* modifies the classical bracket and thereby the corresponding quantum star product – it uses the undamped Hamiltonian, for example. The Dito-Turrubiates proposal is at least economical, since in other formulations involving modified brackets, extra structure must be input. At the end we will discus some emerging problems and possible solutions for them. We will point out what remains to be done and possible future work on the subject.

[1] Some relatively recent works with the latter approach are [49, 42, 34, 9].

4.2 Dissipation – a brief review of quantization techniques

We will present several quantization techniques that share certain features with the deformation quantization method discussed in the next section. Some of those methods may be somewhat limited but they provide a variety of ideas that can be applied in different situations.

4.2.1 Hamiltonian description. Equivalent Hamiltonians

When we deal with classical mechanics we usually think in terms of Hamiltonian mechanics. As we already discussed the Hamiltonian of a closed classical system is the energy of the system and is a conserved quantity. This statement already presents a problem when dissipative systems are involved and energy is lost. If the Hamiltonian still represents the energy of the system then it cannot be a conserved quantity and vice-versa.

We present here the *inverse method of analytical dynamics* applied to the damped harmonic oscillator, i.e. we find the Hamiltonian of the system from the equation of motion. The central question is then how do we find a Hamiltonian for a dissipative system knowing the force that is causing the dissipation or the equations of motion. We will be interested in the damped harmonic oscillator. The equation of motion is

$$\ddot{q} + 2\gamma\dot{q} + \omega^2 q = 0 \tag{4.1}$$

Using the standard Poisson bracket (2.4) we can recover (4.1) if we take either of the

following Hamiltonians[2]:

$$H_1(q,p) = \frac{p^2}{2m}\, e^{-2\gamma t} + \frac{m\omega^2 q^2}{2}\, e^{2\gamma t} \tag{4.2}$$

or

$$H_2(q,p) = -\gamma qp - \ln \frac{\cos(\omega' qp)}{x} \tag{4.3}$$

with $\omega'^2 = \omega^2 - \gamma^2$. From this example we see that a unique way of associating a Hamiltonian to the damped harmonic oscillator might not exist.

To illustrate the problem we consider a force $f(q, \dot{q}, t)$ acting on a single particle moving in one dimension. We assume the Hamiltonian equations

$$\dot{p} = -\partial_q H, \qquad \dot{q} = \partial_p H$$

still hold for dissipative system. Therefore we must recover the Newton's equation

$$m\ddot{q} = f(q, \dot{q}, t). \tag{4.4}$$

if a function is to be the Hamiltonian. In other words we can express the Hamilton equations in terms of the coordinate only and compare with (4.4). That will allow us to write an equation for the Hamiltonian itself

$$\partial^2_{pt} H + \partial^2_{pq} H\ \partial_p H - \partial^2_{pp} H\ \partial_q H = m^{-1} f(q, \partial_p H). \tag{4.5}$$

The equation is highly nonlinear and the general solution is unknown. For a given force Hamiltonians may not exist, a unique Hamiltonian may exist or it might be possible to write an infinite number of them. Even for the simplest systems the problem is very challenging.

[2]For more details refer to [66] - an excellent book on the subject

Different Hamiltonians are by no means physically equivalent. Many of them have unphysical properties and must be rejected. Even when a solution is acceptable as a physical Hamiltonian, it can generate the same motion in the coordinate space but not in the momentum space, i.e. the phase space evolution is not the same. Those are known as *q-equivalent* Hamiltonians. Similarly when the phase space picture is the same for two Hamiltonians they are called *qp*-equivalent. All *q*-equivalent Hamiltonians are related via canonical transformations.

For example (4.2) and (4.3) are both solutions. The asymmetry with respect to time reversal is a feature we would expect from a dissipative Hamiltonian, so they may both generate physically sensible evolution. However if we insist on the interpretation of the Hamiltonian as the energy of the system we must discard H_2 because it is a conserved quantity. On the other hand only H_2 is translationally invariant.

Clearly we can treat dissipative systems in the framework of closed systems. We consider a system of interest A interacting with an environment E and use the Hamiltonian formalism for a closed system. Our purpose here however, is to demonstrate the fact that effective approaches are problematic even at the classical level. This will carry over to the quantum case. In a sense we will have to make choices about which feature are crucial and which are to be abandoned based on physical intuition and following already successful techniques for similar problems. In the end only experiment can tell if an effective approach has merit or not.

4.2.2 Damped-amplified pair of simple harmonic oscillators. Bateman's Hamiltonian

This method for quantization of the damped harmonic oscillator is due to Bateman. He proposes a simple model where we are dealing with two interacting systems, one of which loses energy and the other acquires the same amount of energy from the first one. Since the whole system is closed we can use the Hamiltonian formalism to

describe it without the complications we discussed previously. The entire treatment can be found in [66] in great detail. The proposed Lagrangian has the form

$$L(q_1, \dot{q}_1; q_2, \dot{q}_2) = m\dot{q}_1\dot{q}_2 + m\gamma(q_1\dot{q}_2 - \dot{q}_1 q_2) - m\omega^2 q_1 q_2 \tag{4.6}$$

to recover the equations of motion of a couple of oscillators. The equations of motion are those of the damped harmonic oscillators with different damping constants:

$$m\ddot{q}_1 + 2m\gamma\dot{q}_1 + m\omega^2 q_1 = 0, \tag{4.7}$$

$$m\ddot{q}_2 - 2m\gamma\dot{q}_2 + m\omega^2 q_2 = 0. \tag{4.8}$$

The first equation describes the damped harmonic oscillator as usual. The second equation has the sign of the damping parameter reversed. It describes a system that will acquire energy rather than dissipate it. This way the energy of the system as a whole (both oscillators) is conserved. The two systems are coupled by the dissipation constant (even though the equations are decoupled), much like using normal coordinates for coupled simple harmonic oscillators. The Hamiltonian of the whole system can be obtained from the Lagrangian. It is the well known Bateman Hamiltonian and has the form

$$H(q_1, p_1; q_2, p_2) = \frac{p_1 p_2}{2m} - \gamma(q_1 p_1 - q_2 p_2) + m(\omega^2 - \gamma^2) q_1 q_2 \tag{4.9}$$

The Hamiltonian does not depend on time explicitly and it is a constant of motion $dH/dt = 0$. We will use this Hamiltonian for quantization.

The standard canonical quantization is now performed to find the spectrum. We will use the factorization method that has served us so well in the undamped case. The natural thing to do is to try to rewrite the Hamiltonian as a sum (or in this case difference) of two simple harmonic oscillator Hamiltonians plus a dissipative part

coming from the interaction between them. We can achieve that if we define the ladder operators to be:

$$\hat{a} = (4m\omega\hbar)^{-1/2}[(\hat{p}_1 + \hat{p}_2) - im\omega'(\hat{q}_1 + \hat{q}_2)], \tag{4.10}$$

$$\hat{a}^\dagger = (4m\omega\hbar)^{-1/2}[(\hat{p}_1 + \hat{p}_2) + im\omega'(\hat{q}_1 + \hat{q}_2)], \tag{4.11}$$

$$\hat{b} = (4m\omega\hbar)^{-1/2}[(\hat{p}_1 - \hat{p}_2) - im\omega'(\hat{q}_1 - \hat{q}_2)], \tag{4.12}$$

$$\hat{b}^\dagger = (4m\omega\hbar)^{-1/2}[(\hat{p}_1 - \hat{p}_2) + im\omega'(\hat{q}_1 - \hat{q}_2)]. \tag{4.13}$$

This choice leads to the usual commutation relations between creation and annihilation operators:

$$[\hat{a}, \hat{a}^\dagger] = [\hat{b}, \hat{b}^\dagger] = 1, \quad [\hat{a}, \hat{b}] = [\hat{a}^\dagger, \hat{b}^\dagger] = 0 \tag{4.14}$$

We can express the Hamiltonian in terms of (4.12-4.13) and it assumes the form

$$\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} - \hat{b}^\dagger\hat{b}) + i\hbar\gamma(\hat{a}^\dagger\hat{b}^\dagger - \hat{a}\hat{b}) \tag{4.15}$$

We expect when the dissipation constant is zero to have two independent oscillators. In particular we want the dissipative system (the system of interest) to become the simple harmonic oscillator. Clearly the second term in (4.15) disappears. However we need to set the amplified oscillator in the ground state in order to obtain a simple harmonic oscillator for the dissipative oscillator. In other words if $|n_A, n_B\rangle$ are the eigenvectors for the Bateman Hamiltonian we recover the usual simple harmonic oscillator states if $\hat{b}|n_A, 0\rangle = 0$. Note that without the last condition the Hamiltonian will not be bounded from below for $\gamma = 0$.

Finding the spectrum of the Hamiltonian is not straightforward. However, we can use the Schwinger representation of the angular momentum. A crucial observation will be that the creation and annihilation operators can be combined into operators

with angular momentum-like commutation relations. They are defined as follows

$$\hat{\phi}_0 = (\hat{a}^\dagger \hat{a} - \hat{b}^\dagger \hat{b})/2, \tag{4.16}$$

$$\hat{\phi}_x = (\hat{a}^\dagger \hat{b}^\dagger + \hat{a}\hat{b})/2, \tag{4.17}$$

$$\hat{\phi}_y = i(\hat{a}^\dagger \hat{b}^\dagger - \hat{a}\hat{b})/2, \tag{4.18}$$

$$\hat{\phi}_z = (\hat{a}^\dagger \hat{a} + \hat{b}^\dagger \hat{b})/2. \tag{4.19}$$

The commutation relations are

$$[\hat{\phi}_x, \hat{\phi}_y] = i\hat{\phi}_z, \quad [\hat{\phi}_z, \hat{\phi}_y] = i\hat{\phi}_x, \quad [\hat{\phi}_x, \hat{\phi}_z] = i\hat{\phi}_y. \tag{4.20}$$

The zeroth operator commutes with all the other operators similarly to the magnitude of the angular momentum. A direct calculation shows that

$$\hat{\phi}_0^2 + \frac{1}{4} = \hat{\phi}_z^2 - \hat{\phi}_x^2 - \hat{\phi}_y^2. \tag{4.21}$$

This observation is important since we can now apply techniques that are similar to those already known, i.e. when rotations are involved in quantum mechanics. For this purpose we define the eigenstates for the operators (4.16-4.19) to be

$$\hat{\phi}_0 |jm\rangle = j|jm\rangle, \qquad \hat{\phi}_z |jm\rangle = (m + 1/2)\,|jm\rangle\,. \tag{4.22}$$

The goal is to express the eigenvalues and eigenvectors of the Hamiltonian in terms of (4.22). We substitute the operators in the Hamiltonian to express it in terms of $\hat{\phi}$'s. There is a problem since the Hamiltonian is not directly expressed in terms of

the z-component. Instead we have

$$\hat{H} = 2\hbar\omega\hat{\phi}_0 + 2\hbar\gamma\hat{\phi}_y \,. \tag{4.23}$$

Now we will have to express the eigenstates it in terms of those of $\hat{\phi}_z$. We can check that the following is true using the Baker-Campbell-Hausdorff formula:

$$\hat{\phi}_y = \pm i e^{\mp\pi\hat{\phi}_x/2}\hat{\phi}_z e^{\pm\pi\hat{\phi}_x/2} \,. \tag{4.24}$$

One can now see that the states

$$|\psi^{\pm}_{jm}\rangle = \exp\left(\mp\frac{\pi}{2}\hat{\phi}_x\right)|jm\rangle \tag{4.25}$$

are the eigenstates for the operator $\hat{\phi}_y$:

$$\hat{\phi}_y|\psi^{\pm}_{jm}\rangle = \pm i\,(m+1/2))\,|\psi^{\pm}_{jm}\rangle \,. \tag{4.26}$$

With this relationship we can produce the eigenstates for the Hamiltonian. The equation of motion

$$\hat{H}|\psi^{\pm}_{jm}\rangle = i\hbar\partial_t|\psi^{\pm}_{jm}\rangle \tag{4.27}$$

can be written in terms of the operators $\hat{\phi}$ and that will give us an equation for $|\psi^{\pm}_{jm}\rangle$ which we can solve in terms of $|jm\rangle$

$$|\psi^{\pm}_{jm}\rangle = \exp\left[-2i\omega jt \pm \hbar\gamma(2m+1)t \mp \pi\hat{\phi}_x/2\right]|jm\rangle \,. \tag{4.28}$$

Now let us see what the spectrum of the Hamiltonian looks like. First define the lowering and raising operators as in the simple harmonic oscillator case:

$$\hat{\phi}_{\pm} = \hat{\phi}_x \mp \hat{\phi}_y, \qquad [\hat{\phi}_x, \hat{\phi}_{\pm}] = \pm\hat{\phi}_{\pm} \,. \tag{4.29}$$

The ladder operator can be used to generate the eigenvectors. We expect the spectrum to be bounded so let us assume that for m_0 we have:

$$\hat{\phi}_{\pm}|\psi^{\pm}_{jm_0}\rangle = 0 \tag{4.30}$$

Next we multiply by $\hat{\phi}_{\mp}$ from the left and substitute (4.29) and (4.21) to express the result in terms of $\hat{\phi}_0$ and $\hat{\phi}_y$ as we did for the eigenstates. The result is

$$(1/4 - \hat{\phi}_0^2 - \hat{\phi}_y^2 + i\hat{\phi}_y)|\psi^{\pm}_{jm_0}\rangle = 0\,. \tag{4.31}$$

Acting with operators will result in the relationship between $m_0^2 = j^2$. The ladder operators can then be used to obtain the rest of the values for m

$$m = |j|, |j| + 1/2, |j| + 1, ... \tag{4.32}$$

Comparing our notations $|jm\rangle$ and $|n_A, n_B\rangle$ and recalling that system B has to be in ground state ($|n_A, n_B\rangle = |n_A, 0\rangle$) to recover simple harmonic oscillator for $\gamma = 0$ we can write

$$2j = 2m = n_A := n \tag{4.33}$$

With this in mind we can write the spectrum in terms of one quantum number only:

$$E_n^{\pm} = n\hbar\omega \pm i\hbar\gamma(n+1)\,. \tag{4.34}$$

The Bateman's Hamiltonian is a very informative toy model. Dissipation is regarded as a result of transfer of energy from one part of the system to another. It is exactly solvable and the quantization is standard (although tricky), using canonical quantization without change to the Hamiltonian or the quantization scheme. However the "reservoir" consists of one particle only so the model is mostly of theoretical value.

Also the amplified oscillator must occupy the ground state in order to recover simple harmonic oscillator in the undamped limit. Interestingly, the deformation quantization model presented later shares some of the damped - amplified pair characteristics.

4.2.3 A classical particle coupled to a heat bath. Caldeira-Leggett Hamiltonian

Clearly for any problems of practical interest we must allow a bigger system, a reservoir, to absorb the energy lost from the simple harmonic oscillator. This reservoir can have different physical natures and can be coupled with a system in different way. The physics that follows from that of course will be different. Our goal however is not to describe any particular system but to show that macroscopic dissipation can be recovered from a microscopic Hamiltonian. Also we want to demonstrate the complications that arise even for the simplest classical systems.

We consider a Hamiltonian of the form $H_A + H_E + H_I$, where A is the dissipative system of interest, E is the environment or a reservoir and finally H_I is an interaction Hamiltonian. Physically we are interested in the case of an oscillating particle with quadratic potential. However for now we will allow a more general Hamiltonian as in [76] and [66]

$$H_A = \frac{p^2}{2m} + V(q)\,. \tag{4.35}$$

System A will interact with and transfer energy to the reservoir which consists of N simple harmonic oscillators with a total Hamiltonian

$$H_E = \sum_{i=1}^{N} H_i = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \frac{m_i \omega_i^2 q_i^2}{2}\,. \tag{4.36}$$

The interaction is given in terms of generalized forces and is linear with respect to

the reservoir coordinates:

$$H_I = -\sum_{i=1}^{N} F_i(q)q_i + U(q)\,. \tag{4.37}$$

The "counter-term" included needs to be specified so that the Hamiltonian is translationally invariant (i.e. it counters the breaking of translational symmetry):

$$U(q) = \sum_i \frac{F_i^2(q)}{2m_i\omega_i^2}\,. \tag{4.38}$$

The total Hamiltonian can be written in a simpler form if we assume a *separable interaction* defined as $F_i(q) = c_i F(q)$, i.e. the forces change with q at the same rate for the different particles. Those restrictions result in the so called Caldeira-Leggett Hamiltonian (for linear force):

$$H_{CL} = \frac{p^2}{2m} + V(q) + \frac{1}{2}\sum_{i=1}^{N}\left[\frac{p_i^2}{m_i} + m_i\omega_i^2\left(x_i - c_iF(q)/m_i\omega_i\right)^2\right]\,. \tag{4.39}$$

From this Hamiltonian we can find the equations of motion for the system and the reservoir

$$m\ddot{q} + V'(q) + \sum_{i=1}^{N}\frac{c_i^2F(q)F'(q)}{m_i\omega_i^2} = F'(q)\sum_i c_iq_i\,. \tag{4.40}$$

$$m_i\ddot{q}_i + V'(q) + m_i\omega_i^2q_i = c_iF(q)\,. \quad i \in [0, N] \tag{4.41}$$

This system of equations can be decoupled so that we obtain an equation of motion for the system of interest A only. With the use of the Green's function for (4.41) we can write an explicit solution for the reservoir coordinates

$$q_i(t) = q_{0,i}\cos(\omega_it) + \frac{p_{0,i}}{m_i\omega_i}\sin(\omega_it) + \frac{c_i}{m_i\omega_i}\int_0^t d\tau\,\sin[\omega_i(t-\tau)]F(q(\tau))\,, \tag{4.42}$$

where $q_{0,i}$ and $p_{0,i}$ are the initial conditions for the trajectory of the reservoir in phase

space. After integration by parts we substitute the result in (4.39). Let us now further assume that the force is linear $F(q) = q$. Now the equations for the system A involve the q and its derivatives only:

$$m\ddot{q} + V'(q) + m\int_0^t d\tau\gamma(t-\tau)\dot{q}(\tau) = f(t)\,. \tag{4.43}$$

This is known as the generalized Langevin equation. One of the new quantities involved is the *memory kernel*

$$\gamma(t) = \frac{\theta(t)}{m}\sum_i \frac{c_i^2\cos(\omega_i t)}{m_i\omega_i^2}\,, \tag{4.44}$$

which introduces memory, i.e. dependence on previous times. Another is the *generalized force* coming from the reservoir initial conditions and the linear force in terms of the coefficients c_i

$$f(t) = \sum_i c_i\left[q_{0,i}\cos(\omega_i t) + p_{0,i}\sin(\omega_i t)/m_i\omega_i\right] - m\gamma(t)q(0)\,. \tag{4.45}$$

Classically, the force has zero average value and its correlations, being delta functions, are zero for different times.

To recover the damped harmonic oscillator we must assume the so called *Ohmic damping*, defined as the case when the Fourier transform of the memory kernel is not dependent on the frequency i.e. $\tilde{\gamma}(\omega) = \gamma$. This implies that the memory kernel is a delta function which plugged in the Langevin equation (4.43) gives the classical equation of motion for the damped harmonic oscillator (4.7). Finally we choose all the particles to be originally in their equilibrium state, i.e. the initial conditions $q(0) = q_i(0) = p_i(0)$ will eliminate the force $f(t)$. Of course we can choose any other initial conditions – it will simply result in a different system and not the damped harmonic oscillator.

This a very good example to illustrate the complexity of the problem even at the classical level. The system is closed, the Hamiltonian can be written in terms of operators and standard techniques apply. The quantization then is conceptually clear, however it is technically a difficult problem, considering the size of the reservoir. One can see that the complications coming from the introduction of the reservoir are are sometimes too problematic and even in the case of damped harmonic oscillator it is justified to consider simpler effective treatments.

4.2.4 Complex Hamiltonians

The effective method presented here departs from the canonical formalism in two ways. It involves a complex Hamiltonian and therefore it is not identified with the energy of the system. The phase space coordinates are also complex. The idea was first introduced by Dekker, see [66], for both classical and quantum description. We will present a later result by Rajeev, who revisits Dekker's idea in [65] and provides a different quantization of the damped harmonic oscillator.

The idea is fairly simple. To illustrate let us take a typical Hamiltonian of the form $p^2/2m + V(q)$ and add to the potential energy a complex constant to define a new potential $V_{eff}(0) := V(q) - i\Gamma$. Its easy to see now that the probability to find the particle will decay exponentially:

$$P(t) = \int_{-\infty}^{\infty} |\psi(q,t)|^2 dx = e^{-t/\tau}\,, \tag{4.46}$$

where the decay time τ depends on the constant Γ. Similarly when energy is lost and we expect decaying states we can expect that imaginary parts in the Hamiltonian will cause the decay.

Let us now apply that program to the damped harmonic oscillator. The classical

equations of motion is given, as usual, by

$$\ddot{q} + 2\gamma\dot{q} + \omega^2 q = 0, \quad \gamma > 0\,. \tag{4.47}$$

To switch over to Hamiltonian formalism we rewrite the equation in terms of the phase space coordinates

$$\dot{q} = p, \quad \dot{p} = -2\gamma p - \omega^2 q. \tag{4.48}$$

Strictly speaking this is not a canonical treatment. The "Hamiltonian" is taken as usual to be the energy of the system, $H = p/2m + \omega^2 m^2 q^2/2$, and on the damped trajectory it decreases as time passes, i.e. our system exhibits a physically sensible, dissipative behaviour.

$$\frac{dH}{dt} \propto p\dot{p} + \omega^2 q\dot{q} = -2\gamma p^2 \leq 0\,. \tag{4.49}$$

However H is not a true Hamiltonian because it does not generate the equations of motion using the usual Poisson bracket. We introduce a new set of coordinates

$$z = -iAp + A(\omega_1 - i\gamma)q\,, \tag{4.50}$$

(where A is a normalization constant) and their complex conjugate $\bar{z}$ so that we can write the equations of motion in diagonal form

$$\frac{dz}{dt} = (-\gamma + i\omega_1)z, \quad \omega_1 = \sqrt{\omega^2 - \gamma^2}\,, \tag{4.51}$$

assuming we are only considering the under-damped case.

The Poisson bracket for the canonical variables $\{x, p\} = 1$ becomes $\{z, \bar{z}\} = 2i\omega_1|A|^2$ for the new variables. We can set the normalization so that the bracket is simply $\{z, \bar{z}\} = i$. This starts to remind us of the algebraic method for simple harmonic oscillator and we are going to exploit that similarity. Using the usual

bracket we can recast Hamilton's equation of motion into the usual form if we define the Hamiltonian of the system to be the complex function

$$\mathfrak{H} = (\omega_1 + i\gamma) z\bar{z}\,. \tag{4.52}$$

This form resembles the form of the Hamiltonian when creation and annihilation operators are used. The equations of motion then are the Hamilton equations:

$$\frac{dz}{dt} = \{\mathfrak{H}, z\}, \quad \frac{d\bar{z}}{dt} = \{\mathfrak{H}, \bar{z}\}\,. \tag{4.53}$$

The quantization then follows the spirit of the canonical quantization where we replace the coordinates with operators. Rajeev uses the following rules to associate operators:

$$z \mapsto \hat{a}^\dagger := z, \quad \bar{z} \mapsto \hbar\hat{a} := \hbar\frac{\partial}{\partial z}\,. \tag{4.54}$$

This association leads to the usual commutation relations and to a Hamiltonian that is very similar to the simple harmonic oscillator one:

$$[\hat{a}, \hat{a}^\dagger] = 1, \quad \hat{\mathfrak{H}} = \hbar(\omega_1 + i\gamma)\hat{a}^\dagger\hat{a}\,. \tag{4.55}$$

The anti-Hermitian part is responsible for the dissipation and it disappears when the damping parameter vanishes, as expected.

The eigenvalue equation still makes sense in the non-Hermitian case as long as the Hermitian and anti-Hermitian parts commute. Following the algebraic method as in the simple harmonic oscillator we find that the eigenvalues are given by

$$\mathcal{E}_n = (\omega_1 + i\gamma)n, \quad n \in \mathbb{N}. \tag{4.56}$$

We can use them to write the evolution of a given state:

$$|\psi\rangle = \sum_n \psi|n\rangle \mapsto |\psi\rangle = \sum_n \psi e^{i\hbar\omega_1 nt} e^{-\hbar\gamma nt}|n\rangle. \tag{4.57}$$

In other words this model predicts that every possible state will decay to the ground state if enough time passes. All excited states decay and the more excited the state is the more rapid the decay will be. This is in agreement with physical intuition and is similar to the classical result.

To conclude this section let us refer the reader to [65] and the references therein for further information. Rajeev's work includes comparisons with the Caldeira-Leggett approach.

4.2.5 Quantum maps and Lindblad equation

Rajeev's method deals with a very simple system and the applicability to more complicated and physically interesting systems is still unclear. This section will mostly follow [44], [63] and [57] is an attempt to provide a very brief, simplified and completely self-contained overview of one of the most popular effective approaches - the quantum map approach and the Lindblad equation. This approach is an approximation so we will set the physical restrictions for its applicability. Let us start with evolution of the density operator.

Let us remind that unitary evolution of the density operator of a closed system A with a given Hamiltonian H is given by

$$\hat{\rho}(t+\tau) = \hat{U}(\tau)\hat{\rho}(t)\hat{U}^\dagger(\tau), \quad \hat{U}(\tau) = e^{-i\tau\hat{H}/\hbar}. \tag{4.58}$$

The above equation states that there is a rule, or a *superoperator*, that takes a density operator $\hat{\rho}(t)$ in the past t and transforms it into a density operator $\rho(t+\tau)$ in the

future $t+\tau$. Formally we can write (4.58) as

$$\hat{\rho}(t+\tau) = \Phi_\tau(\hat{\rho}(t))\,. \tag{4.59}$$

Our goal is to generalize that map to include non-unitary evolution of a system A in contact with another system B. A physically meaningful map $\Phi_{A,t}$ is called a *quantum map* and it has to satisfy certain conditions.

1.) A quantum map should be a linear map so that it preserves coherent mixtures of pure states:

$$\Phi_A(a_1\rho_{A,1} + a_2\rho_{A,2}) = a_1\Phi_A(\rho_{A,1}) + a_2\Phi_A(\rho_{A,2})\,. \tag{4.60}$$

This condition is sometimes challenged as too restrictive and one is tempted to include nonlinear maps. However, the nonlinearity needs to be compatible with the probability interpretation which is problematic [63].

Since the quantum map should preserve the set of density operators we need to impose the following

2.) Φ_A transforms a density operator into density operator which is Hermitian. Therefore we need the quantum map to preserve *hermiticity*.

$$(\Phi_A(\hat{\rho}_A))^\dagger = \Phi_A(\hat{\rho}_A)\,. \tag{4.61}$$

3.) A density operator must have an *unit trace* as a consequence of the probability interpretation. Therefore the quantum map needs to preserve that property:

$$\mathrm{Tr}\,(\Phi_A(\hat{\rho}_A)) = 1\,. \tag{4.62}$$

4.) The last condition is *positivity*. The matrix elements of the density matrix are

populations and coherences and therefore positive. This means that for any basis in the Hilbert space $\{|i\rangle_A \in \mathcal{H}_A | i \in I\}$ the matrix elements of the transformed density matrix are non-negative:

$$ {}_A\langle i|\Phi_A(\hat{\rho}_A)|i\rangle_A \geq 0\,. \tag{4.63}$$

Let us now assume that there is a system B that does not interact with A but sometime in the past was entangled with it. The system B is isolated so it does not evolve. At this point this may seem as a very restrictive requirement, since it is possible there are no physical systems that satisfy it. A valid question is whether such setup even exists? The answer is that, at least as an approximation to a physical system, one can find systems that satisfy the above condition. For additional information one can refer to the paragraph in this section, treating the Lindblad equation. We can construct a superoperator that acts on $\hat{\rho}_{AB}$ and describes the evolution of $A + B$. It is reasonable to assume that this superoperator will be $\Phi_A \otimes \mathbf{1}_B$ acting on the density operator in $\mathcal{H}_A \otimes \mathcal{H}_B$. However we cannot claim that the superoperator is a quantum map since it may not preserve the positivity property of the density operator. We must insist on the stronger condition:

$$ {}_{AB}\langle\phi|(\Phi_A \otimes \mathbf{1}_B)(\hat{\rho}_{AB})|\phi\rangle_{AB} \geq 0, \quad \forall\ |\phi\rangle_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B\,. \tag{4.64}$$

The quantum map Φ_A is then called *completely positive* and positivity is usually replaced by complete positivity. More detail can be found in [63] and [44].

Complete positivity is not unanimously accepted as a necessary condition for an evolution superoperator. The reason is that we cannot assume that the physical states are those that lie in the tensor product $\mathcal{H}_A \otimes \mathcal{H}_B$. This assumption must be viewed as an approximation to avoid inconsistencies. In many cases it is justified as we will discuss later in this section. However to assume complete positivity is too restrictive, as pointed out by Pechukas and Weiss, and may lead us to discard important physi-

cally sensible cases. For a full discussion we refer to [61] and [76]. However, complete positivity is a necessary condition for the Lindblad approximation we will use here to derive the Lindblad master equation. Therefore we will use the term quantum map only for completely positive evolution superoperators. Whenever the complete positivity condition cannot be imposed we simply cannot use the Lindblad equation to describe the evolution of the density operator.

Krauss sum representation theorem

We will now show that there is a simple way of writing a completely positive map in a finite dimensional Hilbert space[3]

$$\Phi_A(\rho_A) = \sum_\mu M_\mu \rho_A M_\mu^\dagger \,. \tag{4.65}$$

Let us have two systems A and B with Hilbert spaces $\mathcal{H}_I,\ \dim \mathcal{H}_I = N_I,\ I = A, B$. Assume they are originally entangled in the state expressed in an orthogonal basis:

$$|\Psi\rangle_{AB} = \sum_i |i\rangle_A \otimes |i\rangle_B \,, \tag{4.66}$$

a pure state from the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. This means that A is not entangled with the environment initially. Now we assume that we have taken B far away and we have put A in contact with the environment. We can now express the evolution of the system in terms of the quantum map $\Phi_A \otimes \mathbf{1}_B$ since the system B is not evolving. Now we can show that there is a way to express the quantum map Φ_A acting on A only in terms of $\Phi_A \otimes \mathbf{1}_B$.

To do that let us define *partial inner product* as a map $\mathcal{H}_A \otimes \mathcal{H}_B \mapsto \mathcal{H}_A$

$$|\phi\rangle_A = {}_B\langle\phi^*|\psi\rangle_{AB} \,, \tag{4.67}$$

[3]We consider finite dimensional space for simplicity. For the case of infinite dimensional Hilbert space one can refer to the original paper: [57] which treats the more general case.

where the state $|\phi^*\rangle_B$ is called *index state* and it produced by the anti-linear map:

$$|\phi\rangle_A = \sum_i a_i |i\rangle_A \mapsto |\phi^*\rangle_B \stackrel{\text{def}}{=} \sum_i \bar{a}_i |i\rangle_B \,. \tag{4.68}$$

Here it is now apparent that we will need to prepare a system B for which $N_A \leq N_B$ so that the map is injective. Now let us apply the quantum map $\Phi_A \otimes \mathbf{1}_B$ to a pure state $|\Psi_{AB}\rangle$:

$$\begin{aligned}(\Phi_A \otimes \mathbf{1}_B)(|\Psi\rangle_{AB}\langle\Psi|_{AB}) &= (\Phi_A \otimes \mathbf{1}_B) \sum_{ij} |i\rangle_A\langle j|_A \otimes |i\rangle_B\langle j|_B \\ &= \sum_{ij} \Phi_A(|i\rangle_A\langle j|_A) \otimes |i\rangle_B\langle j|_B \,,\end{aligned} \tag{4.69}$$

where we use normalization ${}_{AB}\langle\Psi|\Psi\rangle_{AB} = N_A$. We use $\langle i|_A$ and ${}_A\langle i|$ indiscriminately, depending on the situation. Now we use an arbitrary index state $|\phi^*\rangle_B = \sum_i \bar{a}_i |i\rangle_B$ to "sandwich" the density operator in (4.69), using the partial inner product (4.67) much like when we evaluate the matrix elements of an operator:

$$\sum_{ij} \Phi_A(|i\rangle_A\langle j|_A) \sum_{k,l} a_k \, {}_B\langle k|i\rangle_B \; \bar{a}_l \, {}_B\langle j|l\rangle_B = \Phi_A(|\phi\rangle\langle\phi|) \,. \tag{4.70}$$

The other portion of the equation (4.69) is simply $\langle\phi^*|(\Phi_A \otimes \mathbf{1}_B)|\Psi\rangle_{AB\,AB}\langle\Psi|\phi^*\rangle$. This leads to the expression for the quantum map of A only from the full quantum map

$$\Phi_A(|i\rangle_A\langle j|_A) = {}_B\langle\phi^*| \left[(\Phi_A \otimes \mathbf{1}_B)(|\Psi\rangle_{AB}\langle\Psi|_{AB}) \right] |\phi^*\rangle_B \,. \tag{4.71}$$

Now let us remember that the state we chose is described by a density operator and so is its image under the quantum map. Therefore it can be written as an ensemble of pure states $|\Phi_\mu\rangle_{AB}\langle\Phi_\mu|_{AB}$ with associated probabilities P_μ, i.e.:

$$\Phi_A(|\phi\rangle_A\langle\phi|_A) = \sum_\mu P_\mu \; {}_B\langle\phi^*|\Phi_\mu\rangle_{AB} \; {}_{AB}\langle\Phi_\mu|\phi^*\rangle_B \,. \tag{4.72}$$

The last step is to notice that the map

$$M_\mu : |\phi\rangle_A \mapsto \sqrt{P_\mu}\ {}_B\langle\phi^*|\Phi_\mu\rangle_{AB} \tag{4.73}$$

is linear and therefore defines an operator in $\mathcal{H}_A$. We can extend this linearity for density matrices that do not represent pure states by the linearity of the quantum map. Finally the trace preserving property of the quantum map will lead to:

$$\sum_\mu \hat{M}_\mu \hat{M}_\mu^\dagger = \hat{\mathbf{1}}_A \,. \tag{4.74}$$

Note that this argument requires complete positivity of Φ_A in order to claim that $\Phi_A \otimes \mathbf{1}_B$ is positive and therefore the image of a density operator is still a density operator and therefore can be written as in (2.50). Also it depends on the assumption that a quantum map is linear. The Krauss sum representation is crucial for the Lindblad equation so let us rewrite (4.65) more explicitly to use it later

$$\hat{\rho}(t+\tau) = \Phi_{A,\tau}(\hat{\rho}(t)) = \sum_\mu \hat{M}_\mu(\tau)\hat{\rho}(t)\hat{M}_\mu^\dagger(\tau) \,. \tag{4.75}$$

The Lindblad master equation

The quantum map program may have a lot of merit to it but it is difficult to apply in practical calculations. In practice we need an algorithm to find the density operator of a given system usually by solving a differential equation. The Krauss sum representation may be a remarkable result but not very helpful because the operators in the sum depend on the final time in the evolution. We will now show that with the help of the Krauss sum we can derive a differential equation for the density operator. We have to keep in mind that in order for that equation to have physical meaning we might only be justified in applying it when certain conditions are met.

We expect the equation of motion for non-unitary evolution to be a generalization

of those for the unitary case

$$\frac{d\hat{\rho}(t)}{dt} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}]\,. \tag{4.76}$$

Therefore we expect the equations to be of first order with respect to time. This means that the evolution is local in time. Physically, we can only apply local equations to a system for which we can ignore the memory effects. Crudely speaking we can ignore the memory effects when the system's evolution is such that the time it takes to go back into the equilibrium state is much larger than the typical time needed for the system A to interact with the reservoir E. On the other hand we need that time to be very small compared to the overall time. Then we can write

$$\frac{d\hat{\rho}_A(t)}{dt} = \frac{\hat{\rho}_A(t+\tau) - \hat{\rho}_A(t)}{\tau} = \frac{\Phi_{A,\tau}(\hat{\rho}_A(t)) - \hat{\rho}_A(t)}{\tau}\,. \tag{4.77}$$

This cannot be taken to be exact as a $\lim_{\tau\to\infty}$ for the reasons stated above but is still a good approximation for very small time increments in the above sense. Approximation that is local in time is called "Markovian". A big system E will have a wide energy range $\Delta E = \hbar\Delta\omega$ ([44] and [21]). The correlation time τ_c is of order $\hbar/\Delta\omega$. Markov approximation implies $\tau_c \ll T$, where T is the time scale of the observables' evolution. According to [44], if V is the order of the matrix elements of H_{AE}, the Markovian evolution $\tau_c \ll T$ is guaranteed when $\tau_c \ll \hbar/V$.

For the quantum map in the above equation to reproduce $\rho_A(t)$ we need one of the operators to be of zeroth order in terms of τ:

$$\hat{M}_0 = \hat{\mathbf{1}} - i\hat{K}\tau + \mathcal{O}(\tau^2), \qquad \hat{K} = \hbar^{-1}\hat{H} - i\hat{J} \tag{4.78}$$

Here $\hat{K}$ is just any operator that is constant with respect to τ (of course it does not depend on t either). We split into its Hermitian and anti-Hermitian part. Keeping only the fist order terms we can substitute the operator $\hat{M}_0$ into the Krauss sum

representation so we get:

$$\hat{M}_0\hat{\rho}_A\hat{M}_0^\dagger = \hat{\rho}_A - \frac{i\tau}{\hbar}[\hat{H},\hat{\rho}_A] - \tau(\hat{J}\hat{\rho}_A + \hat{\rho}_A\hat{J}) \tag{4.79}$$

This sorts out the zeroth term and the first term coming from $\hat{M}_0$. However there is a first order contribution from all the other operators $\hat{M}_\mu,\ \mu \neq 0$ therefore we can write them as $\hat{M}_\mu = \sqrt{\tau}\hat{L}_\mu$, where the operators $\hat{L}_\mu$ do not depend on τ. Now we apply the normalization condition which written in terms of the new operators is

$$\sum_\mu \hat{M}_\mu\hat{M}_\mu^\dagger = \hat{\mathbf{1}} - 2\tau\hat{J} + \tau\sum_{\mu\neq 0}\hat{L}_\mu^\dagger\hat{L}_\mu = \hat{\mathbf{1}} \tag{4.80}$$

which allows us to find $\hat{J}$ in terms of $\hat{L}_\mu$:

$$\hat{J} = \frac{1}{2}\sum_{\mu\neq 0}\hat{L}_\mu^\dagger\hat{L}_\mu. \tag{4.81}$$

Plugging (4.81) and (4.79) in (4.77) we get the Lindblad equation:

$$\frac{d\hat{\rho}_A(t)}{dt} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}_A] + \sum_{\mu\neq 0}\left(\hat{L}_\mu\hat{\rho}_A(t)\hat{L}_\mu^\dagger - \frac{1}{2}\hat{L}_\mu^\dagger\hat{L}_\mu\hat{\rho}_A(t) - \frac{1}{2}\hat{\rho}_A(t)\hat{L}_\mu^\dagger\hat{L}_\mu\right) \tag{4.82}$$

Let us note that the Lindblad equation depends crucially on the existence of the Krauss representation. The Krauss representation in turn depends on the factorization of the density operator. In other words we assume

$$\hat{\rho}_{AE}(t) = \hat{\rho}_A(t)\otimes\hat{\rho}_E \tag{4.83}$$

with $\hat{\rho}_E$ unchanging under the interaction between the two systems. Clearly this is not the case in general. The dissipative system is in generally entangled with the

environment and the density operator can be written as

$$\hat{\rho}_{AE} = \hat{\rho}_A(t) \otimes (\hat{\rho}_E + \delta\hat{\rho}_E(t)) + \delta\hat{\rho}_{AE}(t). \tag{4.84}$$

However if the system E is big enough so that its fluctuation $\delta\hat{\rho}_E(t)$ is negligible and also the coupling is weak enough so that correlation $\delta\hat{\rho}_{AE}(t)$ is negligible then the factorization (4.83) will be well justified.

The environment fluctuation and and the correlation between the two systems have correlation time that is of order τ_c so if we restrain the applicability of the Lindblad equation to a coarse-grained time evolution where the time scale $\tau \gg \tau_c$ the high frequency oscillations will not influence the evolution since the effects will only be noticeable at shorter times, i.e. $\tau_c \ll \tau \ll T$.

4.3 The damped harmonic oscillator in phase-space quantum mechanics

We start in this section with a review of the Dito and Turrubiates [32] model of damping in a quantum harmonic oscillator in phase space, with comments added. A new contribution will then be described: our incorporation of Wigner functions and their evolution. First, a naïve proposal will be examined, and rejected, since it leads to an unacceptable evolution equation. The equation of motion will then be modified, and explained. Finally, its consequences are outlined. One such consequence is that the Wigner function of the damped harmonic oscillator follows the canonical flow. This property is also common to all non-dissipative systems having quadratic Hamiltonians, including the simple (undamped) harmonic oscillator. Since the damped and undamped harmonic oscillator and such systems are treated similarly in some other approaches, this seems physically reasonable.

4.3.1 Dissipation as deformation of the Poisson bracket

Dito and Turrubiates [32] describe the damped harmonic oscillator using the Hamiltonian of the undamped simple harmonic oscillator. In a sense then, they describe its dissipation as kinematics. More precisely, the dissipation is encoded in a deformation of the classical Poisson bracket of the harmonic oscillator and its consequent quantum $*$-product.

The initial observation is that the classical equations of motion of the damped harmonic oscillator can be written as

$$\dot{q} \;=\; \{q, H\}_\gamma \;=\; p/m \;;\;\; \dot{p} \;=\; \{p, H\}_\gamma \;=\; -m\omega^2 q \;-\; 2\gamma p \tag{4.85}$$

using the *undamped* Hamiltonian $p^2/2m + m\omega^2 q^2/2$. The price paid is that we must use a deformed Poisson bracket

$$\begin{aligned} \{\, f, g \,\}_\gamma \;&:=\; \{f, g\} \;-\; 2\gamma m\, \partial_p f\, \partial_p g \\ &=\; f \left(\overleftarrow{\partial}_q \overrightarrow{\partial}_p \;-\; \overleftarrow{\partial}_p \overrightarrow{\partial}_q \;-\; 2\gamma m \;\overleftarrow{\partial}_p \overrightarrow{\partial}_p \right) g \;, \end{aligned} \tag{4.86}$$

with the damping constant γ as deformation parameter. Notice that the deformed bracket is no longer skew,[4] and doesn't obey the Jacobi identity (and therefore is not a product in a Lie algebra).

This proposal certainly makes sense at classical level. The energy of the system can still be given by the Hamiltonian except now it will not be conserved on the classical trajectory as in [65]:

$$\frac{dH}{dt} = \{q, H\}_\gamma = -\frac{2\gamma}{m} p^2(t) \leq 0 \,. \tag{4.87}$$

[4] The deformed bracket can be obtained from the Poisson bracket by the substitutions $\overleftarrow{\partial}_q \to \overleftarrow{\partial}_q - 2\alpha m\gamma \overleftarrow{\partial}_p$ and $\overrightarrow{\partial}_q \to \overrightarrow{\partial}_q + 2\beta m\gamma \overrightarrow{\partial}_p$, for any real α and β such that $\alpha + \beta = 1$. The sign difference in front of γ between the substitutions for the left- and right-acting derivatives foreshadows our proposal (4.124).

Moreover for a physical observable given by $t \mapsto f_t(q,p)$ we have the usual form of the equation of motion, except the Poisson bracket is now replaced by the modified bracket:

$$\frac{df_t(q,p)}{dt} = \frac{df(q(t),p(t))}{dt} = \{f,H\}_\gamma(q(t),p(t))\,. \tag{4.88}$$

This result applies to a general class of classical systems: if we use any Hamiltonian of the form

$$\tilde{H} \;=\; \frac{p^2}{2m} \;+\; V(q)\;, \tag{4.89}$$

with an arbitrary potential $V(q)$, the same damping term $2m\gamma\dot{q}$ is still the only modification of the equation of motion for $q(t)$. We will restrict attention here to the simple harmonic oscillator and its damped version, however.

4.3.2 The star-gamma product and Dito-Turrubiates' treatment of damped harmonic oscillator

Just as the Moyal product is related to the Poisson bracket, the Dito-Turrubiates damped $*$-product is obtained by exponentiation of the deformed classical bracket (4.86):

$$*_\gamma \;:=\; \exp\Big[\,\frac{i\hbar}{2}(\overleftarrow{\partial}_q\overrightarrow{\partial}_p - \overleftarrow{\partial}_p\overrightarrow{\partial}_q - 2\gamma m\,\overleftarrow{\partial}_p\overrightarrow{\partial}_p)\Big] \;=\; *\,e^{-i\hbar\gamma m\overleftarrow{\partial}_p\overrightarrow{\partial}_p}\;. \tag{4.90}$$

Why exponentiate? In the undamped case, it is necessary for the homomorphism of the $*$-algebra with the operator algebra. Also, the Moyal $*$-product is the unique associative deformation of the point-wise multiplication of functions on $\mathbb{R}^{2n}$, up to isomorphism (by transition operators – see below). No similar result for the damped product is known; neither is the operator algebra for the damped case. Exponentiation is therefore an assumption.

On the other hand, suppose that we posit

$$*_\gamma \;:=\; F\left(\frac{i\hbar}{2}(\overleftarrow{\partial}_q\overrightarrow{\partial}_p - \overleftarrow{\partial}_p\overrightarrow{\partial}_q - 2\gamma m\,\overleftarrow{\partial}_p\overrightarrow{\partial}_p)\right)\,, \tag{4.91}$$

for some function F. Since $\{\cdot,\cdot\}_\gamma \to \{\cdot,\cdot\}$ as $\gamma \to 0$, requiring that $\lim_{\gamma\to 0} *_\gamma = *$ selects the exponential function. The possibility that the form (4.91) is too restrictive remains, however.

We can derive an integral representation for the $*_\gamma$-product just like in the undamped case. Using the integral representation we find that the $*_\gamma$-product defers from the Moyal product by a correction in the symplectic volume term:

$$\begin{aligned}(f*_\gamma g)(q,p) = \int \frac{dq'dq''dp'dp''}{\pi^2} f(q',p')g(q'',p')\times \\ \exp\Big\{-2i\big[p(q'-q'')+p'(q''-q)+p''(q-q')\big]\Big\}\exp\Big\{-4i\gamma(q''-q)(q'-q)\Big\}\end{aligned} \tag{4.92}$$

One key result of [32] is

$$T(\,f\,*\,g\,)\;=\;(Tf)*_\gamma(Tg)\,, \tag{4.93}$$

with

$$T\;=\;\exp\Big(\frac{-i\hbar m\gamma}{2}\,\partial_p^2\Big)\,. \tag{4.94}$$

To show this we use that the relationship between equivalent $*$-products $\tilde{T}(f*g) = (Tf)\tilde{*}(Tg)$ can be rewritten using the Leibniz rule to read

$$\tilde{*} = *\tilde{T}^{-1}[\overleftarrow{\partial}]\tilde{T}[\overleftarrow{\partial}+\overrightarrow{\partial}]\tilde{T}^{-1}[\overrightarrow{\partial}], \tag{4.95}$$

where $\overleftarrow{\partial}$ stands for either $\overleftarrow{\partial}_p$ or $\overleftarrow{\partial}_q$,

$$\tilde{T}[\overleftarrow{\partial}+\overrightarrow{\partial}] := \tilde{T}\big|_{\partial\to\overleftarrow{\partial}+\overrightarrow{\partial}} \tag{4.96}$$

and similarly for $T^{-1}[\overleftarrow{\partial}]$ and $\tilde{T}^{-1}[\overrightarrow{\partial}]$. That is, the Dito-Turrubiates damped star product is c-equivalent to the Moyal star product. As discussed in the previous section, c-equivalence does not imply physical equivalence, and so the damped star product has the potential to describe the dissipation of a damped harmonic oscillator.

So, what effect does the Dito-Turrubiates transition operator T have? First, it is clear that T does more than change the ordering, since it has no fixed bi-grade in the powers of p and q. Its effect is therefore more profound. An important example is

$$T\left(\frac{p^2}{2m} + V(q)\right) = \frac{p^2}{2m} + V(q) - i\frac{\hbar\gamma}{2}\,; \tag{4.97}$$

(see also (4.106)).[5] T transforms a real Hamiltonian into a complex one.

For such a conversion to be possible, it is necessary, but not sufficient, that $\overline{T} \neq T$. Another consequence of a non-real transition operator is that $*_\gamma$ is not Hermitian:

$$\overline{a *_\gamma b} = \overline{b} *_{-\gamma} \overline{a} \neq \overline{b} *_\gamma \overline{a}\,. \tag{4.98}$$

Its c-equivalence with the Moyal star product ensures that the damped star product $*_\gamma$ is associative, for any value of the damping constant γ. For example, $*_{-\gamma}$ will be useful later because of (4.98), and it is also associative. However, problems exist if any two different damping parameters γ and γ' are used. Care must be taken with regard to the order of multiplications. Clearly,

$$f *_\gamma (1 *_{\gamma'} g) \neq (f *_\gamma 1) *_{\gamma'} g\,, \tag{4.99}$$

if $\gamma \neq \gamma'$, for example. A unique product such as $a *_\gamma b *_{-\gamma} c$ does not (automatically) exist.

[5] This last result is also interesting in its own right, since it recalls a different approach to damped systems that uses complex Hamiltonians (see [28, 66], and also [65]).

Use of a naïve substitution

$$\{a,b\}_\gamma \stackrel{?}{\to} \frac{[\,a\,,\,b\,]_{*_\gamma}}{i\hbar} \tag{4.100}$$

leads to

$$0 \;=\; \frac{\partial \rho_\gamma}{\partial t} \;+\; \frac{1}{i\hbar}[\rho_\gamma, H]_{*_\gamma}\;, \tag{4.101}$$

where ρ_γ indicates the Wigner function of the *damped* harmonic oscillator. This equation of motion integrates to

$$\rho_\gamma(p,q;t) \;=\; U_\gamma(p,q;t) *_\gamma \rho_\gamma(p,q;0) *_\gamma U_\gamma(p,q;-t)\;. \tag{4.102}$$

Here

$$U_\gamma(p,q;t) \;:=\; \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{-itH}{\hbar}\right)^{*_\gamma n} \;=\; \mathrm{Exp}[*_\gamma]\left(\frac{-itH}{\hbar}\right) \tag{4.103}$$

satisfies the damped analogue of (2.100), i.e.

$$i\hbar\partial_t\, U_\gamma(p,q;t) \;=\; H *_\gamma U_\gamma(p,q;t)\;. \tag{4.104}$$

Dito-Turrubiates solve (4.104), without discussing the evolution of Wigner functions. They then Fourier-Dirichlet expand the solution to find the spectrum of eigenvalues and eigenfunctions of

$$H *_\gamma \rho_{\gamma,E} \;=\; E_\gamma\, \rho_{\gamma,E}\;. \tag{4.105}$$

Using (5.11), one finds

$$\begin{aligned} U_\gamma(p,q;t) \;&=\; \mathrm{Exp}[*_\gamma]\left(\frac{-itH}{\hbar}\right) \;=\; T\Big(\,\mathrm{Exp}[*]\left(\frac{-itT^{-1}(H)}{\hbar}\right)\,\Big) \\ &=\; T\Big(\,\mathrm{Exp}[*]\left(\frac{-it[H+i\hbar\gamma/2]}{\hbar}\right)\,\Big) \;=\; e^{\gamma t/2}\,T\Big(U(p,q;t)\Big)\;. \end{aligned} \tag{4.106}$$

Using the explicit form for the $*$-exponential

$$U(q,p;t) = \frac{1}{\cos(\omega t/2)} \exp\left\{ \frac{2H \tan(\omega t/2)}{i\hbar\omega} \right\} \tag{4.107}$$

and (4.94), this gives [32]

$$\begin{aligned} U_\gamma(p,q;t) \;&=\; \frac{\exp(\gamma t/2)}{\cos(\omega t/2)\left[1+\frac{2\gamma}{\omega}\tan(\omega t/2)\right]} \\ &\times \exp\left\{ \frac{2\tan(\omega t/2)}{i\hbar\omega} \left(\frac{p^2}{2m[1+\frac{2\gamma}{\omega}\tan(\omega t/2)]} \;+\; \frac{1}{2}m\omega^2 q^2 \right) \right\} \;. \end{aligned} \tag{4.108}$$

Using the equivalence operator T and the spectral decomposition of (4.107) we find the expansion of U_γ

$$\mathrm{Exp}[*_\gamma] \left(\frac{-itH}{\hbar} \right)(q,p) \;= \exp(\gamma t/2) \sum_{n=0}^{\infty} \exp[-i(n+1/2)\omega t] T(\rho_{E_n}) \,. \tag{4.109}$$

That gives the solutions of (4.105) in terms of the simple harmonic oscillator analogues and the corresponding energies:

$$\rho_{\gamma,n} \;=\; T\left(\rho_{E_n}\right) \;, \tag{4.110}$$

with

$$E_{\gamma,n} \;=\; E_n \;+\; i\frac{\hbar\gamma}{2} \;=\; \frac{\hbar}{2}\left[(2n+1)\omega \;+\; i\gamma\right] \;. \tag{4.111}$$

The spectrum is now complex which is a result of the non-Hermitian nature of the $*_\gamma$-product. It will correspond to a non-Hermitian Hamiltonian in operator representation. For example, for $n=0$ Dito and Turrubiates [32] find

$$\begin{aligned} \rho_{E_{\gamma,0}} \;&=\; \frac{2}{\sqrt{1-2i\gamma/\omega}} \\ &\times \exp\left\{ -\frac{2}{\hbar\omega} \left(\frac{p^2}{2m[1-2i\gamma/\omega]} \;+\; \frac{1}{2}m\omega^2 q^2 \right) \right\} \;. \end{aligned} \tag{4.112}$$

We can find the rest of the states alternatively using the familiar factorization method. First we express the Hamiltonian using the holomorphic and anti-holomorphic variables with the help of the $*_\gamma$-product

$$H = \hbar\omega(\bar{a} *_\gamma a + 1/2 + i\gamma/2\omega). \tag{4.113}$$

The $*_\gamma$-commutation relations are similar to the simple harmonic oscillator ones:

$$[a, H]_{*_\gamma} = -i\omega a, \quad [\bar{a}, H]_{*_\gamma} = i\omega\bar{a}, \quad [a, \bar{a}]_{*_\gamma} = 1/i\hbar\,. \tag{4.114}$$

Now we can write the general solution as $\rho_{E_n E_m} = \underbrace{\bar{a}*_\gamma ...*_\gamma \bar{a}}_{n \text{ times}} *_\gamma \rho_0 *_\gamma \underbrace{a*_\gamma ...*_\gamma a}_{m \text{ times}}$. However these Wigner functions' complex values present an physical interpretation problem.

4.3.3 Problems associated with the $*_\gamma$-product quantization. Modified equations of motion.

Dito-Turrubiates' treatment is simple and elegant but it has two serious flaws. There is a fundamental problem with the basic equation of motion, eqn. (4.101). For the damped harmonic oscillator it yields

$$0 \;=\; \frac{\partial\rho_\gamma}{\partial t} \;+\; \frac{1}{i\hbar}[\rho_\gamma, H]_{*_\gamma} \;=\; \frac{\partial\rho_\gamma}{\partial t} \;+\; \frac{1}{i\hbar}[\rho_\gamma, H]_{*} \;+\; i\gamma\hbar\,\partial_p\partial_q\rho_\gamma\;. \tag{4.115}$$

Notice that the term proportional to the damping constant γ is not real. But the eigenvalues of the density matrix are the populations, and they must be real. Time evolution must preserve the reality of the density matrix. The imaginary damping term in (4.115) means that a real density matrix does not remain real as it evolves.

An equally important flaw is revealed by the limit

$$\lim_{\hbar\to 0} \frac{1}{i\hbar}[H, \rho_\gamma]_{*_\gamma} \;=\; \{H, \rho_\gamma\} \;\neq\; \{H, \rho_\gamma\}_\gamma\;. \tag{4.116}$$

This is a direct consequence of the c-equivalence of $*_\gamma$ and $*$. But this shows that there is no damping in the classical limit. The classical limit of (4.101) is not correct!

To try to understand better the origin of the difficulties with the purported equation of motion (4.101), let us consider how it might be "derived". Notice that (4.101) would result from the undamped evolution equation (4.76) by the substitution

$$\rho_\gamma \stackrel{?}{=} T(\rho) \ , \tag{4.117}$$

a generalization of (4.110). This simple identification is appealing in part because it is similar to

$$\rho_H(q,p;t) = T_H \rho(q,p;t) \tag{4.118}$$

used to define the Husimi phase-space distribution $\rho_H(p,q;t)$. Recall that the Husimi distribution does not encode the same physics as the Wigner function. The explicit form of (4.118)

$$\rho_H(q,p;t) = \frac{1}{\pi\hbar}\int dp'dq'\rho(q',p';t)\exp\left\{-\frac{1}{\hbar}\left[\frac{(q-q')^2}{s^2} + s^2(p-p')^2\right]\right\} \tag{4.119}$$

indicates that the Husimi distribution is a smoothed version of the Wigner function, coarse grained by a squeezed[6] Gaussian weighting in phase space. Also recall that we need to use a c-equivalent star product - the Husimi star product $*_H$ - instead of Moyal star- product. The Husimi equation of motion is found directly from that for the Wigner function, by substituting (4.118). Additional terms arise in the Husimi equation of motion compared to that for the Wigner function, since the coarse-graining evolves in time [70]. Just as the "twisting" by T_H modifies the equation of motion, so does application of the Dito-Turrubiates transition operator

[6]More precisely, the distribution functions for general s were introduced in [16], [**?**], while the Husimi distribution has s=1. We call the Gaussian weighting of (4.119) squeezed because it is proportional to the Wigner transform of a squeezed state.

T. The physical damping is meant to be introduced that way.

Following (4.119), one might hope for an interpretation of $T(\rho)$ as the Wigner distribution coarse-grained in momentum space. That point of view is not sensible, however, since the weighting would have to be Gaussian-like with an imaginary exponent. This does point to the origin of the main problem, however: unlike the Husimi transition operator T_H, the Dito-Turrubiates T is not real.

As a consequence, eqn. (4.97) can hold: T transforms a real Hamiltonian into a complex one. That is the crucial point here, we believe. Compare to a similar situation – if a non-self-adjoint Hamiltonian is used, the equation of motion of the density operator is modified,[7] to

$$0 \;=\; i\hbar\,\frac{\partial\hat{\rho}}{\partial t} \;+\; \hat{\rho}\,\hat{H} \;-\; \hat{H}^{\dagger}\,\hat{\rho}\;. \tag{4.120}$$

By analogy, we should consider [8]

$$-\,i\hbar\,\frac{\partial\rho_\gamma}{\partial t} \;=\; \rho_\gamma *_\gamma H \;-\; \overline{\rho_\gamma *_\gamma H}\;. \tag{4.121}$$

Notice that the right-hand side of this equation is purely imaginary, so that

$$\frac{\partial\rho_\gamma}{\partial t} \;=\; -\,\frac{2}{\hbar}\,\mathrm{Im}\,(\,\rho_\gamma *_\gamma H\;)\;. \tag{4.122}$$

This implies that the reality of the Wigner function

$$\rho_\gamma \;=\; \overline{\rho_\gamma} \tag{4.123}$$

[7] See [36], for example, where the analogous modified equation of motion for a Heisenberg operator was shown to lead to a quantum anomaly.

[8] This form may possibly be related to the bi-orthogonal quantum mechanics discussed by Curtright and Mezincescu [25]. For related work in phase space, see [27] and [67].

is preserved in evolution.[9] We can therefore also write

$$-\,i\hbar\,\frac{\partial\rho_\gamma}{\partial t}\;\;=\;\;\rho_\gamma *_\gamma H\;\;-\;\;H\;*_{-\gamma}\;\rho_\gamma\;. \tag{4.124}$$

With this prescription it is easy to show that the classical limit makes sense for the simple harmonic oscillator Hamiltonian:

$$\lim_{\hbar\to 0}\;\frac{\rho_\gamma *_\gamma H\;-\;H\;*_{-\gamma}\;\rho_\gamma}{i\hbar}\;=\;\frac{\{\rho_\gamma, H\}_\gamma\;-\;\{H,\rho_\gamma\}_{-\gamma}}{2}\;=\;\{\rho_\gamma, H\}_\gamma\;. \tag{4.125}$$

We emphasize that the relation (4.117) is then *not* obeyed.

Let us now attempt to argue for (4.124) from other grounds. As a starting point, let us assume that the Liouville Theorem still holds, and try to modify the argument that led to

$$i\hbar\frac{\partial\rho}{\partial t}+[\rho,H]_*=0 \tag{4.126}$$

to justify the damped equation of motion (4.124). An important advantage of the Dito-Turrubiates method is that it only modifies the classical brackets. That advantage would be lost if we need to input something to replace the Liouville Theorem. Therefore, we assume the equation of motion is

$$\frac{d\rho_{\gamma,c}}{dt}\;\;=\;\;\frac{\partial\rho_{\gamma,c}}{\partial t}\;\;+\;\;\{\,\rho_{\gamma,c}, H\,\}_\gamma\;\;=\;\;0\;. \tag{4.127}$$

The phase-space version of the Dirac quantization rule $\{a,b\}\;\rightarrow\;[a,b]_*/i\hbar$ above should therefore be deformed to

$$\{a,b\}_\gamma\;\;\rightarrow\;\;\frac{a *_\gamma b\;-\;\overline{a *_\gamma b}}{i\hbar}\;\;=\;\;\frac{a *_\gamma b\;-\;b\;*_{-\gamma}\;a}{i\hbar} \tag{4.128}$$

for real observables a and b, in order to recover the equation of motion (4.121).

[9] According to (4.122), if ρ_γ had a non-zero imaginary part, it would not evolve.

One might be tempted to write

$$\rho_\gamma(p,q;t) \stackrel{?}{=} U_\gamma(p,q;t) *_\gamma \rho_\gamma(p,q;0) *_{-\gamma} \overline{U_\gamma(p,q;t)} \tag{4.129}$$

as a real solution to the equation of motion (4.124). But this expression is ambiguous at best, as shown by the discussion around eqn. (4.99).

Luckily, however, a formal solution to (4.124) *can* be written, by deforming the undamped solution of

$$i\hbar\frac{\partial\rho}{\partial t} = ad_H[*]\rho := i\hbar\mathcal{L}\rho \tag{4.130}$$

written as

$$\rho(q,p;t) = \exp\left\{-\frac{it}{\hbar}ad_H[*]\right\}\rho(q,p;0) = \exp\{t\mathcal{L}\}\,\rho(q,p;0) \tag{4.131}$$

where we define $ad_f[*]g := [f,g]_*$s. If we define

$$\mathrm{ad}_*^{(\gamma)}[f]\,g \;:=\; f *_{-\gamma} g \;-\; g *_\gamma f \;, \tag{4.132}$$

then (4.124) is

$$i\hbar\,\frac{\partial\rho_\gamma}{\partial t} \;=\; \mathrm{ad}_*^{(\gamma)}[H]\,\rho_\gamma \;=:\; i\hbar\mathcal{L}_\gamma\,\rho_\gamma \;. \tag{4.133}$$

The solution is just

$$\rho_\gamma(p,q;t) \;=\; \exp\left\{\,\frac{-it}{\hbar}\,\mathrm{ad}_*^{(\gamma)}[H]\,\right\}\,\rho_\gamma(p,q;0) \;=\; \exp\{\,t\,\mathcal{L}_\gamma\,\}\;\rho_\gamma(p,q;0)\;. \tag{4.134}$$

There is no associative ambiguity in this explicit solution.

A more explicit result can be given immediately for the damped harmonic oscillator, having

$$\mathcal{L}_\gamma \;=\; m\omega^2 q\,\frac{\partial}{\partial p} \;-\; \frac{p}{m}\left(\frac{\partial}{\partial q} \;-\; 2m\gamma\frac{\partial}{\partial p}\right)\;. \tag{4.135}$$

The quantum evolution is (4.124), but that reduces to (4.127), with $\rho_{\gamma,c} \to \rho_\gamma$. The quantum Wigner function satisfies the classical equation of motion. The Wigner function at time t is therefore simply

$$\rho_\gamma(p,q;t) \;=\; f\,(\,p_c(-t),q_c(-t)\,)\;\;, \tag{4.136}$$

where $p_c(t)$ and $q_c(t)$ characterize the classical (damped) trajectories in phase space. Thus the quantum damped harmonic oscillator follows the classical backward flow of the phase-space coordinates. Perhaps this is not surprising, since for any quadratic Hamiltonian, such as that of the undamped simple harmonic oscillator, the same results holds (see [79], e.g.).

4.4 Discussion and open questions regarding $*_\gamma$-product and dissipation

The presented methods of quantization have their merits and disadvantages. Dissipative systems in quantum mechanics are difficult to treat. Nevertheless physical systems with dissipation are successfully quantized in the operator and path integral approaches. Deformation quantization, therefore, has to be able to provide a phase space quantization version of dissipative systems. This important for two reasons – first, to test deformation quantization as an alternative quantization technique. Secondly, to check if the unique features of deformation quantization will make the description of dissipative systems easier. Let us summarize.

We have shown how to describe the dynamics of Wigner functions in the Dito-Turrubiates scheme [32]. The non-Hermitian damped star product $*_\gamma$ is c-equivalent to the Moyal product $*$. Therefore, if the evolution equation of the damped Wigner function only involves $*_\gamma$-commutators, only Poisson brackets survive in the classical

limit, rather than the damped bracket $\{\cdot,\cdot\}_\gamma$. The classical limit would then be damping-free, and therefore incorrect.

However, the damped transition operator T transforms the simple harmonic oscillator Hamiltonian into a complex one, according to (4.97). Consequently, the evolution equation does not involve $*_\gamma$-commutation, but must instead be (4.124). This ensures that a real Wigner function remains real as it evolves, and the classical limit is correct. Not only is the classical limit correct, it is exact. The damped harmonic oscillator in this formalism therefore follows the classical flow, a property shared with non-dissipative systems in phase space having quadratic Hamiltonians.

Most helpful to us were (i) comparisons of the damped star product $*_\gamma$ with other physical star products that are also c-equivalent to the Moyal $*$, viz. the standard product $*_S$, and the Husimi product $*_H$; and (ii) the Heisenberg equation of motion for an operator observable modified for a non-Hermitian Hamiltonian (see [36], e.g.).

Let us now conclude with a few of the many questions that remain. We hope progress can be made toward their answers.

Should the damped $*_\gamma$-product be obtained by exponentiating $i\hbar\{\cdot,\cdot\}_\gamma/2$? In the case at hand, much of the structure of the γ-deformed star product is irrelevant. Since we use the quadratic Hamiltonian $p^2/2m + m\omega^2 q^2/2$, the only terms that enter are those that are up to quadratic in $\overleftarrow{\partial}$ and $\overrightarrow{\partial}$. In this sense, our main result has a certain robustness. More work on this question would be helpful, however.

Is there a deformed structure analogous to the Heisenberg-Weyl group that is relevant to the damped case? In the undamped case, the Heisenberg-Weyl group is the structure of paramount importance. The Moyal $*$-product simply provides a $*$-realization of that group. As discussed around (4.99), associativity can be a problem in the damped case. But if (4.134) is an appropriate guide, perhaps

$$\exp\Big\{\,\mathrm{ad}_*^{(\gamma)}[ap+bq]\,\Big\}\;e^{cp+dq} \;=\; e^{cp+dq}\,e^{-i\hbar(ad-bc+2m\gamma ac)} \tag{4.137}$$

can serve the purpose. Here a, b, c and d are constants, so that e^{ap+bq} and e^{cp+dq} $*$-represent elements of the Heisenberg-Weyl group. When $\gamma \to 0$ in (4.137), a form of the defining $*$-relations of the Heisenberg-Weyl group is recovered.

Can a solution to the damped equation of motion (4.124) analogous to the undamped formula

$$\rho(q,p;t) = \sum_{E,E'} R_{E,E}(0) \exp\left[\frac{-i(E-E')t}{\hbar}\right] \rho_{E,E'}(q,p)$$

be written? It is clear from (4.134) that the $*$-eigen equation of $\mathrm{ad}_*^{(\gamma)}[H]$ is relevant, so one can start there. One possible ansatz follows, although it may only have relevance for very small γ. Suppose we find the time-independent off-diagonal Wigner matrix elements $\rho_{\gamma;\mathcal{E},\mathcal{E}'} = \rho_{\gamma;\mathcal{E},\mathcal{E}'}(p,q)$ satisfying

$$H *_{-\gamma} \rho_{\gamma;\mathcal{E},\mathcal{E}'} = \overline{\mathcal{E}}\, \rho_{\gamma;\mathcal{E},\mathcal{E}'} , \quad \rho_{\gamma;\mathcal{E},\mathcal{E}'} *_{\gamma} H = \mathcal{E}'\, \rho_{\gamma;\mathcal{E},\mathcal{E}'} , \tag{4.138}$$

where the complex eigenvalues[10] are

$$\mathcal{E} = E + i\lambda , \quad \mathcal{E}' = E' + i\lambda' , \tag{4.139}$$

with $E, E' \in \mathbb{R}$, and $\lambda, \lambda' \in \mathbb{R}_+$. If the real eigenfunctions of (4.138) exist and are complete at all times t, then we can expand

$$\rho_\gamma(p,q;t) = \sum_{\mathcal{E},\mathcal{E}'} R_{\mathcal{E},\mathcal{E}'}(t)\, \rho_{\gamma;\mathcal{E},\mathcal{E}'}(p,q) . \tag{4.140}$$

[10] For the role such complex eigenvalues play in another description of the damped harmonic oscillator, see [19]. Wigner functions involving such eigenvalues are considered in [18].

The equation of motion then yields

$$\begin{aligned}\rho_\gamma(p,q;t) &= \sum_{\mathcal{E},\mathcal{E}'} R_{\mathcal{E},\mathcal{E}'}(0)\,\exp\left[\frac{-i(\overline{\mathcal{E}}-\mathcal{E}')t}{\hbar}\right]\,\rho_{\gamma;\mathcal{E},\mathcal{E}'}(p,q) \\ &= \sum_{\mathcal{E},\mathcal{E}'} R_{\mathcal{E},\mathcal{E}'}(0)\,\exp\left[\frac{-i(E-E')t}{\hbar}\right]\,\exp\left[\frac{-(\lambda+\lambda')t}{\hbar}\right]\,\rho_{\gamma;\mathcal{E},\mathcal{E}'}(p,q)\ . \qquad (4.141)\end{aligned}$$

If this conjecture is correct, then the physically important $*$-eigen equations are those given in (4.138). It would not be clear then that the phase-space functions of (4.110) are directly relevant.

The ansatz of (4.138-4.141) reduces to the undamped system when $\hbar \to 0$. It is also devoid of unphysical stationary states – the imaginary parts of eigenvalues λ and λ' *both* contribute to the damping of the dynamics. Furthermore, the system is consistent with (4.136) if $(\overline{\mathcal{E}}-\mathcal{E}')/\hbar$ is independent of $\hbar$. Such eigenvalues were obtained in [32], as indicated in (4.111). However, the corresponding solutions (4.110) are not real – see (4.112), e.g.

Can the Dito-Turrubiates scheme be related to other quantization methods for dissipative systems (see [28, 66, 75])? Certainly, hints of connections with other models are apparent. For example, Dekker's use of a complex Hamiltonian is recalled by $T(H) = H - i\hbar\gamma/2$. Bateman's doubled system of a damped and anti-damped oscillator comes to mind from $\mathrm{ad}_*^{(\gamma)}[H]\rho = H*_\gamma\rho - \rho *_{-\gamma} H$; in this last expression, however, the anti-damped ($\gamma \to -\gamma$) system is dual rather than extra/auxiliary. The importance of resonances has been emphasized by [18, 19] and others, and seems relevant to the $*_\gamma$- and $*_{-\gamma}$-eigen equations of the previous paragraph. Finally, if the correspondence (4.117) were correct, then we would be able to define a damped Wigner transform

$$\mathcal{W}_\gamma \ := \ T^{-1}\,\mathcal{W} \ = \ \mathcal{W}\,\hat{T}^{-1}\ , \qquad (4.142)$$

where

$$\hat{T}^{-1} \;=\; \exp\left\{ -\frac{im}{2\hbar}\left(\mathrm{ad}[\hat{x}]\right)^2 \right\}. \tag{4.143}$$

The form of this $\hat{T}$ appears to be consistent with Tarasov's [72] proposal to include superoperators in the operator formulation of quantum mechanics in order to adapt it to dissipative systems.

Can other dissipative physical systems be treated in a similar way? One very useful example might be spin systems, with relaxation.

Instead of dissipation, might other physical effects, such as decoherence, be describable in the Dito-Turrubiates manner?

Chapter 5

Conclusion

Let us conclude this thesis with a concise account of our results, and a discussion of our expectations and open questions. We pushed the limits of deformation quantization applying it to two extreme types of systems where quantization is subtle in general. Let us start with contact interactions.

Robin boundary conditions for the infinite wall potential

In [5] and [6] we considered the infinite wall in relation to deformation quantization. In addition to pure deformation quantization problems we obtained results that are valid in quantum mechanics in general regardless of the approach used. These results along with a short treatment of background material were presented in chapter three of this thesis.

Let us remind that for systems with boundaries or discontinuous potentials the symbol of the density operator does not satisfy the $*$-eigenvalue equations for the bulk Hamiltonian. As a consequence if we solve the $*$-eigenvalue equations we cannot perform matching as in operator quantum mechanics. One way of resolving this problem is to modify the Hamiltonian. Equivalently, we can replace the $*$-eigenvalue equations with higher order ones, to account for the interaction introduced by the

boundaries. Our treatment is based on the understanding that in quantum mechanics discontinuous potentials are only idealizations of physical potentials – the discontinuous potentials only have physical meaning as limits of smooth potentials. In the case of the infinite wall potential we can take the limit of the Liouville potential (3.85):

$$\lim_{\alpha\to\infty} \frac{\hbar^2\kappa^2}{2m}\, e^{-2\alpha q} \ . \tag{5.1}$$

Quantization of this potential is possible, however it only realizes the standard wall. The Robin boundary conditions (3.28)

$$\psi(0) \ + \ L\,\psi'(0) \ = \ 0, \quad L \neq 0 \tag{5.2}$$

are not realized. We can use the Šeba potential (3.34), but it is discontinuous and therefore will not be convenient for deformation quantization. The Morse potential (3.45) is a generalization of the Liouville potential and it resembles the shape of the Šeba potential:

$$V_M(q) \ = \ \frac{\hbar^2\kappa^2}{2m}\, \left(e^{-2\alpha q} - b\ e^{-\alpha q} \right) \ . \tag{5.3}$$

This potential recovers the nonstandard walls in the limit $\alpha \to \infty$ as long as the parameters are taken to be

$$b = \ (2n+1) - \ 2L^{-1}/\alpha \ + \ \mathcal{O}(\alpha^{-2}) \ , \quad \kappa = \alpha \, . \tag{5.4}$$

The constant b can assume only very limited values or (5.3) recovers the standard wall just as the Liouville potential does. This choice of a very special form is known as "fine tuning" and it has been observed for the Šeba and finite step potentials. The finite discrete part is similar to the cases when Šeba finite step potential are used. The infinitesimal, α-dependent part is an addition specific to the Morse potential only.

The physical significance of the fine tuning is that it selects a resonance. At energies that select the fastest change in the phase, in the $\alpha \to \infty$ limit, the fine-tuning condition (3.38) is recovered. We expect that the Morse potential shares that property.

Let us point out that now we can see that (5.3) has explicit mass dependence. We need different potentials for particles with different masses. Again, the above mentioned potentials share this property, as well.

Let us consider deformation quantization now. The symbol of the density matrix for Robin boundary conditions is (3.122)

$$\rho(q,p) \propto \frac{\sin\left[2(p/\hbar - k)q\right]}{(p/\hbar - k)} + \frac{\sin\left[2(p/\hbar + k)q\right]}{(p/\hbar + k)} + 2\cos(2kq - \delta_k)\frac{\sin\frac{2}{\hbar}p\,q}{p/\hbar}\ . \qquad (5.5)$$

However this Wigner function does not satisfy the $*$-eigenvalue equations in the bulk. One can recover this result using pure deformation quantization of the Morse potential (5.3) for a finite α

$$\rho_{k_L k_R}(q,p) \propto \int_{c-i\infty}^{c+i\infty} ds\left(16e^{4\alpha q}\right)^{-s} w_L(s,k_L)\, w_R(s,k_R)\ . \qquad (5.6)$$

with $w_L(s,k_L)$ and $w_R(s,k_R)$ given by (3.124) and (3.125), and taking the limit $\alpha \to \infty$. The limit of this Wigner function is (5.5) similarly to the operator mechanics case.

Finally let us recap. Non-standard walls can be realized as a limit of the Morse potential. This way in deformation quantization we can quantize first and then take the $\alpha \to \infty$ limit, thus avoiding the original problem. Mass dependence and fine tuning may arise but they have their physical explanation in terms of reflection resonance. It is now clear that Dirichlet boundary conditions are called standard since they occur in all cases except for a very limited subset of the values of the parameters.

Let us now discuss some open questions in relation to contact interactions. It

is not clear in general that the fine tuning and the mass dependence are inevitable when discontinuous potentials are modeled by smooth ones. An integrable finite smooth potential would be interesting to be worked out, perhaps for the finite step using a tanh-potential. For finite potentials we can apply the integral form of the equations (2.116) and compare with the existing approaches. They should, at least in principle, agree and point us towards a Dias-Prata type solution but from within the deformation quantization framework. On the other side the infinite wall is special, since it is not an integrable function and the integral equations will not hold. It is therefore desirable to compare sharp finite potentials with sharp infinite potentials.

Deformation quantization of the damped harmonic oscillator

The fourth chapter contains the treatment of the damped harmonic oscillator. The work of Dito and Turrubiates [32] introduces a treatment of the classical oscillator using a modification of the Poisson bracket:

$$\{ f, g \}_\gamma = f \left(\overleftarrow{\partial}_q \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_q - 2\gamma m \overleftarrow{\partial}_p \overrightarrow{\partial}_p \right) g \, , \tag{5.7}$$

Just as the Poisson bracket is responsible for the evolution of a closed system the γ-deformed bracket determines the classical motion for the damped harmonic oscillator

$$\dot{q} = \{q, H\}_\gamma = p/m \, ; \quad \dot{p} = \{p, H\}_\gamma = -m\omega^2 q - 2\gamma p \, . \tag{5.8}$$

This bracket leads to the equation of motion of the damped Harmonic oscillator with Hamiltonian $p^2/2m + m\omega^2 q^2/2$, i.e. unmodified simple harmonic oscillator one.

Similarly to (2.31), define a $*_\gamma$-product by exponentiating the γ-deformed bracket (4.90)

$$*_\gamma := \exp \left[\frac{i\hbar}{2} (\overleftarrow{\partial}_q \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_q - 2\gamma m \overleftarrow{\partial}_p \overrightarrow{\partial}_p) \right] . \tag{5.9}$$

It is a product related to the Moyal $*$-product via

$$*_\gamma = * \, e^{-i\hbar\gamma m \overleftarrow{\partial}_p \overrightarrow{\partial}_p} \tag{5.10}$$

and moreover it is a c-equivalent to the Moyal $*$-product. Recall that means that an invertible operator exists that satisfies

$$T(\, f \, * \, g \,) \;=\; (Tf) *_\gamma (Tg) \;, \tag{5.11}$$

with

$$T \;=\; \exp\Big(\frac{-i\hbar m\gamma}{2} \, \partial_p^2 \Big) \;. \tag{5.12}$$

This new $*_\gamma$-product is used to quantize the system – to find Wigner functions, energies, etc.

However the Dito-Turrubiates methods suffers two shortcomings. Firstly, the classical limit (4.116) is wrong:

$$\lim_{\hbar\to 0} \frac{1}{i\hbar}[H, \rho_\gamma]_{*_\gamma} \;=\; \{H, \rho_\gamma\} \;\neq\; \{H, \rho_\gamma\}_\gamma \;. \tag{5.13}$$

This simply means that in the classical limit the dissipation disappears which contradicts the starting point. Secondly the equations of motion

$$0 \;=\; \frac{\partial \rho_\gamma}{\partial t} \;+\; \frac{1}{i\hbar}[\rho_\gamma, H]_{*_\gamma} \;=\; \frac{\partial \rho_\gamma}{\partial t} \;+\; \frac{1}{i\hbar}[\rho_\gamma, H]_{*} \;+\; i\gamma\hbar \, \partial_p \partial_q \rho_\gamma \tag{5.14}$$

contain an imaginary damping term which means that a real density matrix does not remain real as it evolves. This is also physically unacceptable. So how do we fix these two problems without changing the spirit of this method, which is using the $*_\gamma$-product.

Let us consider operator quantum mechanics and a Hamiltonian that is not self

adjoint. The equation of motion for a density operator will have the form

$$0 \;=\; i\hbar\,\frac{\partial\hat{\rho}}{\partial t} \;+\; \hat{\rho}\,\hat{H} \;-\; \hat{H}^{\dagger}\,\hat{\rho}\;. \tag{5.15}$$

This points to the modification of equations of motion

$$-\,i\hbar\,\frac{\partial\rho_{\gamma}}{\partial t} \;=\; \rho_{\gamma} *_{\gamma} H \;-\; H *_{-\gamma} \rho_{\gamma}\;. \tag{5.16}$$

needed in order to obtain the classical limit $[\rho_{\gamma}, H]_{\gamma} \to \{\rho_{\gamma}, H\}_{\gamma}$. Also it preserves the reality of the Wigner functions as one can see from the following

$$\frac{\partial\rho_{\gamma}}{\partial t} \;=\; -\,\frac{2}{\hbar}\,\mathrm{Im}\,(\,\rho_{\gamma} *_{\gamma} H\;)\;. \tag{5.17}$$

As Dito-Turrubiates' and our work shows, deformation quantization is applicable in systems with dissipation. The damped harmonic oscillator treatment shows that dissipation can be introduced in a very economical way, by further deforming the algebra of observables with the dissipation parameter added to the Planck's constant as a second deformation parameter. Also the Wigner function is preferable to the density operator in many cases. While this example may be just a toy model, we believe that deformation quantization and the Wigner function are a natural setting for systems with dissipation. More complicated phenomena could be include by modifying the Hamiltonian and the $*$-product even further. In general, however it is interesting how different $*$-products may reproduce different physical phenomena? How general is this program? Is it always an effective approach, applicable only within certain limitations or is there a more general underlying structure to be explored?

Outside of the scope of this thesis remain many topics related to deformation quantization. While non-relativistic quantum mechanics is almost fully developed in the bosonic case, fermionic $*$-products are still actively studied. Different $*$-products

are extensively used in relation to quantum field theory, string theory, etc. both in the mathematical and physical literature. The elegant geometric formulation of deformation quantization may provide valuable insight in those areas, where the more familiar approaches are not straightforward.

In conclusion, deformation quantization clearly has a lot to offer in terms of ideas, unique relation to its classical limit, calculational power and interpretation. Generalizations of the star products discussed here, are increasingly used in string theory, noncommutative geometry, etc. It is a field of research that is expanding quickly and will provide a lot of open questions for future research.

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Appendices

Appendix A

Darboux construction of Wigner functions for Morse potential

In the third chapter we found the Wigner functions for a very general family of Morse potentials. In this appendix we will do the same for a special case of the Morse potential using a different technique. The method is directly adapted from supersymmetric quantum mechanics[1] and can be used in operator or deformation quantization in almost identical fashion, the relation being the Wigner-Weyl correspondence. However we are only interested in the calculational aspect of it, and in particular, in what is known as Darboux construction.

Let us consider a single particle Hamiltonian on the real line in operator quantum mechanics:

$$\hat{H}_1 = \frac{\hat{p}^2}{2m} + V_1(\hat{q})\,. \tag{A.1}$$

A general Hamiltonian may factorized in two operators in a way similar to the algebraic method for simple harmonic oscillator:

$$\hat{H}_1 = \hat{A}^\dagger \hat{A}, \quad \hat{A} = \frac{i\hbar}{2m}\frac{d}{dq} + W(q), \quad \hat{A}^\dagger = -\frac{i\hbar}{2m}\frac{d}{dq} + W(q)\,. \tag{A.2}$$

The operators can be determined by comparing with (A.1). That leads to the identification:

$$V_1(q) = W^2(q) - \frac{\hbar}{\sqrt{2m}}W'(q)\,. \tag{A.3}$$

The differential equation is known as Riccati equation and a formula exist to be recast in a more manageable second order linear equation, namely the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\partial_q^2\psi_0 + V_1(q)\psi_0 = 0 \tag{A.4}$$

with the use of the substitution

$$W(q) = -\frac{\hbar}{\sqrt{2m}}\frac{\psi_0'(q)}{\psi_0(q)}\,. \tag{A.5}$$

[1]For an exhaustive review of the subject refer to [22].

This reflects the fact that when the ground state $\psi_0(q)$ has zero energy $E_0^{(1)} = 0$, no nodes and its zero at $\pm\infty$ we can find the potential

$$V_1(q) = \frac{\hbar^2}{2m}\frac{\psi_0''(q)}{\psi_0(q)}\,. \tag{A.6}$$

An important observation is that when we find a state that satisfies $\hat{A}\psi_0 = 0$ we actually find a solution to the Schrödinger equation for zero energy: $H_1\psi_0(q) = \hat{A}^\dagger\hat{A}\psi_0(q) = 0$. Then is a trivial matter to find the function $W(q)$ using the equation (A.5). $W(q)$ is called *superpotential*.

Now why is that an useful endeavor? Note that if we know the whole spectrum $E_n^{(1)}$ of $\hat{H}_1$ and the corresponding wave functions $\psi_n^{(1)}(q)$, $(n \in \mathbb{N})$ then any function

$$\psi_n^{(2)} = \hat{A}\psi_n^{(1)}(q) \tag{A.7}$$

will be a solution to the Schrödinger equation for a different Hamiltonian

$$\hat{H}_2 = \hat{A}\hat{A}^\dagger = \frac{\hat{p}^2}{2m} + V_2(q) \tag{A.8}$$

where the second Hamiltonian is now obtained via an equation very similar to (A.3):

$$V_2(q) = W^2(q) + \frac{\hbar}{\sqrt{2m}}W'(q)\,. \tag{A.9}$$

Of course this it is now trivial to find the potential $V_2(q)$ since we are not solving a differential equation. Let us see how the tho operators and their eigenfunctions and eigenvalues are related:

$$\hat{H}_1\psi_n^{(1)} = E_n^{(1)}\psi_n^{(1)} \tag{A.10}$$

$$\hat{H}_2\hat{A}\psi_n^{(1)} = \hat{A}\hat{A}^\dagger\hat{A}\psi_n^{(1)} = E_n^{(1)}(q)\hat{A}\psi_n^{(1)}\,. \tag{A.11}$$

Since the ground state is annihilated by the operator $\hat{A}$ the ground state for $\hat{H}_2$ will be the first nontrivial state namely $\hat{A}\psi_1^{(1)}$. Therefore the two Hamiltonians are almost isospectral due to the fact that the ground state for the original Hamiltonian does not have a corresponding eigenstate of the SUSY partner Hamiltonian except $\psi_0(q)$. The connection between the different states for the two are given by:

$$\begin{aligned}
\psi_n^{(2)} &= \frac{\hat{A}\psi_{n+1}^{(1)}}{\sqrt{E_n^{(1)}}}\,, \\
\psi_n^{(1)} &= \frac{\hat{A}^\dagger\psi_{n-1}^{(2)}}{\sqrt{E_{n-1}^{(2)}}}\,, \\
E_n^{(2)} &= E_{n+1}^{(1)}, \quad E_0^{(1)} = 0\,.
\end{aligned} \tag{A.12}$$

Before we turn to Wigner functions let us point out that supersymmetry had nothing to do with this brief review. However this property of the Hamiltonians

can be understood from the underlying algebraic structure. Since it is beyond the scope of this work we are only going to show how to relate the Darboux construct to supersymmetry but we encourage the interested reader to look for more information in [22] and the references therein.

Let us now construct the operators:

$$\mathbf{H} := \begin{pmatrix} \hat{H}_1 & 0 \\ 0 & \hat{H}_1 \end{pmatrix}, \quad \mathbf{Q} := \begin{pmatrix} 0 & 0 \\ \hat{A} & 0 \end{pmatrix}, \quad \mathbf{Q}^\dagger := \begin{pmatrix} 0 & \hat{A}^\dagger \\ 0 & 0 \end{pmatrix}, \tag{A.13}$$

Now we can reproduce all the commutation and anticommutation relations to recognize the superalgebra $sl(1/1)$:

$$[\mathbf{H}, \mathbf{Q}] = [\mathbf{H}, \mathbf{Q}^\dagger] = \{\mathbf{Q}, \mathbf{Q}\} = \{\mathbf{Q}^\dagger \mathbf{Q}^\dagger\} = 0\,, \tag{A.14}$$

$$\{\mathbf{Q}, \mathbf{Q}^\dagger\} = \mathbf{H}\,. \tag{A.15}$$

How supersymmetry is responsible for the isospectral property, shape invariance and much more can be found in [22].

Let us turn our attention back to deformation quantization. The Darboux method was first applied to deformation quantization in [24]. Consider the symbol of the Hamiltonian and factorize with respect to the star product in the algebra of phase space functions:

$$H_1 = \frac{p^2}{2m} + V_1(q) = \bar{A} * A \tag{A.16}$$

with the factorizing functions being the corresponding symbols from the operator version. Now comparing as before:

$$\frac{p * p}{2m} + iW(q) * \frac{p}{\sqrt{2m}} - i\frac{p}{\sqrt{2m}} * W(q) + W(q) * W(q) = H_1\,. \tag{A.17}$$

This lead us back to equation (A.3) and the corresponding Schrödinger equation. This is the second time a Schrödinger equation emerges naturally from deformation quantization. We have to be careful because the interpretation following (A.4) will not be valid here since the states are not the wave functions but the Wigner functions. Now lets take a Wigner function $\rho(q,p)$ that is an $*$-eigen function of the Hamiltonian H_1. It is straightforward to check that $A * \rho * \bar{A}$ is a $*$-eigen function of the partner Hamiltonian $A * \bar{A}$ for the same energy. There are analogous formulae to the ones in the operator case. All can be trivially found or Wigner-Weyl transformed directly from the operator versions. We will no proceed to the quantization for Morse potential as an example for Darboux construction.

Deformation quantization of Morse potential from Liouville potential

In this section we are going to Work out a particular case of the family of Morse potentials (3.45). In general a Morse potential has another Morse potential for superpartner. Therefore only a degenerate Morse potential recovering a Liouville potential

will be easier to work out. Therefore we will start with the Morse potential and see when the superpartner is Liouville using the table in [33]. The superpotential for Morse is

$$W(q) = A - Be^{-\alpha q}\,. \tag{A.18}$$

We can therefore compute the two superpotentials:

$$V_1(q) = B^2 e^{-2\alpha q} - \left(2AB + \hbar B\alpha/\sqrt{2m}\right) e^{-\alpha q} + A^2, \tag{A.19}$$

$$V_2(q) = B^2 e^{-2\alpha q} - \left(2AB - \hbar B\alpha/\sqrt{2m}\right) e^{-\alpha q} + A^2. \tag{A.20}$$

Setting $A = \hbar\alpha/\sqrt{8m}$ we get a Liouville potential and $B = \hbar\alpha/\sqrt{2m}$ will turn $V_2(q)$ in the form (3.45) up to a constant term:

$$V_L(q) = \frac{\hbar^2\alpha^2}{2m}\left(e^{-2\alpha q} + 1/4\right)\,, \tag{A.21}$$

$$V_M(q) = \frac{\hbar^2\alpha^2}{2m}\left(e^{-2\alpha q} - 2e^{-\alpha q} + 1/4\right)\,. \tag{A.22}$$

It is now clear that the Liouville potential will provide us with solutions for the Morse potential via the simple relationship (A.12). The Liouville states have already been found (e.g. see [24]) so all we need to do is strip the constant when we find the states for (A.22) and we will find the states for (3.45) when $b = 2$.

$$\psi_L(q) \propto K_{\frac{i}{\alpha}\sqrt{\frac{2mE}{\hbar^2} - \frac{\alpha^2}{4}}}\left(e^{-\alpha q}\right)\,. \tag{A.23}$$

Now using (A.12) we can find the Morse wave functions (unbound) and setting $\nu := \frac{i}{\alpha}\sqrt{\frac{2mE}{\hbar^2} - \frac{\alpha^2}{4}}$:

$$\psi_M(q) = \left(e^{-\alpha q} - \nu - \frac{1}{2}\right) K_\nu\left(e^{-\alpha q}\right) + e^{-\alpha q} K_{\nu+1}\left(e^{-\alpha q}\right)\,. \tag{A.24}$$

Stripping the extra $\alpha^2/4$ coming from the constant term we arrive at the solution for (3.45). Very similarly we can find the Wigner functions for Morse form the Wigner function for Liouville (3.94). The calculation is long but straightforward. We calculate explicitly the $*$-products in $\rho_m(q,p) = \bar{A} * \rho_L * A$ or alternatively we transform the wave functions using the Wigner-Weyl correspondence. In both cases we get the result given by (3.114) for $b = 2$. A direct check shows that while calculationally heavy and long this solution is trivially found.

Appendix B

Phase space for particle with spin from the orbit method

In the second chapter we chose the sphere as the phase space for particles with spin. The sphere is a symplectic manifold that has a Lie group acting on it that leaves the symplectic form invariant. A possible motivation for the choice of phase space comes from the orbit method.

The orbit method is also important because it can be used to find the equivalence classes of unitary irreducible representations of Lie groups. We cannot cover the orbit method here since whole books are written on the subject. A very complete and understandable account of the orbit method can be found in the book [51]. More condensed version of the book can be found in [50]. Also [73] has an interesting non-rigorous treatment of the orbit method in the case of infinite dimensional Lie algebras. The orbit method works best for nilpotent groups. Nevertheless it is still applicable for compact Lie groups, non-compact Lie groups, infinite dimensional or quantum groups – more generally all cases in which the notion of coadjoint orbits makes sense.

However, we are more interested in the fact that a Lie group will naturally act on the coadjoint orbits in precisely the way we described earlier, with a symplectic form arising naturally from the Lie group structure. It is then easy to identify the phase spaces with the coadjoint orbits for a particular symmetry Lie group. The orbit method is used in [8] to describe open strings. In [15] the spin particle is treated as an example of a more general program – a particle with phase space a symplectic manifold with invariance group a Lie group preserving the symplectic structure. Finally [39] treats several examples with different Lie groups.

Here we will provide the derivation of the sphere as a coadjoint orbit and hence a phase space, i.e. symplectic manifold invariant under the $SU(2)$ group. Those details were omitted in the introduction chapter. They are provided here for the sake of clarity and completeness. We will find the symplectic forms of the orbits explicitly for $SU(2)$. The method works with minimal changes for any compact Lie group.

Let us consider $SU(2,\mathbb{C})$ – the Lie group of all 2×2 unitary matrices with unit determinant. Imposing those conditions we find the general form of an element of the

group is:

$$g(u,v) = \begin{pmatrix} u & v \\ -\bar{v} & \bar{u} \end{pmatrix}, |u|^2 + |v|^2 = 1\,. \tag{B.1}$$

The Lie algebra of $SU(2)$ is denoted by $\mathfrak{su}(2)$ and is the algebra of 2×2 traceless anti-Hermitian matrices. For our purposes $SU(2) = \exp\{\mathfrak{su}(2)\}$. Let us consider the basis[1]

$$X = \frac{i}{2}\sigma^2 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},\ Y = \frac{i}{2}\sigma^1 = \frac{1}{2}\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix},\ Z = \frac{i}{2}\sigma^3 = \frac{1}{2}\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \tag{B.2}$$

Therefore an element

$$A(x,y,z) = xX + yY + zZ = \frac{1}{2}\begin{pmatrix} iz & x+iy \\ -x+iy & -iz \end{pmatrix}. \tag{B.3}$$

We can define duality via the linear functional $F(X) \stackrel{\text{def}}{=} \mathrm{Tr}(FX)$. The dual $\mathfrak{su}(2)^*$ space is isomorphic to $\mathfrak{su}(2)$, so the covectors will look the same as the vectors. Let us now find the dual basis $\{F_j\}_{j=1,3}$ to $\{X,Y,Z\}$ (also we use $X_i,\ i=1,2,3$ respectively) using the definition $\langle F_i, X_j\rangle = \delta_{ij}$, where the action is defined as

$$\langle F_i, X_j\rangle \stackrel{\text{def}}{=} F_i(X_j) \ \text{ and } \ F_1(X) \stackrel{\text{def}}{=} \mathrm{Tr}(F\cdot X)\,. \tag{B.4}$$

The last definition can be applied to Y and Z as well. Explicitly the action definition and the duality condition produce a system of linear equations for the matrix elements of F_1. The same type of calculation gives us the other two co-vectors. Therefore, we find that the dual basis is

$$F_1 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},\ F_2 = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix},\ F_3 = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}. \tag{B.5}$$

The generic dual element then is given as the matrix:

$$F(a,b,c) = aF_1 + bF_2 + cF_3 = \begin{pmatrix} -ic & -a-ib \\ a-ib & ic \end{pmatrix}. \tag{B.6}$$

to recover the appearance of the usual euclidean scalar product:

$$\langle F, A\rangle = \mathrm{tr}(F\cdot A) = ax + by + cz. \tag{B.7}$$

To find the coadjoint orbits we use that the exponentiation of the algebra recovers the connected part of the group that contains the unit element. A general element can be written as a composition of the type[2]

$$g(\alpha,\beta,\gamma) = \exp(\alpha X)\exp(\beta Y)\exp(\gamma Z)\,. \tag{B.8}$$

[1]The multiplicative constants are chosen for convenience – the imaginary unit is in order for the basis to be anti-Hermitian and 1/2 is customary in the physics notation.

[2]The exponentiation should be of the generic element $xX+yY+zZ$. However any factors arising from commutation relations will involve exponents of the basis. In fact going from $\exp(xX+yY+zZ)$ to (B.8) is equivalent to a change of local coordinates on the group manifold.

Let us first determine the action of the one-parameter elements. We explicitly compute the exponent that has $\beta = \gamma = 0$:

$$g_\alpha \stackrel{\text{def}}{=} g(\alpha, 0, 0) = \exp(\alpha X) = \begin{pmatrix} \cos\frac{\alpha}{2} & \sin\frac{\alpha}{2} \\ -\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{pmatrix}. \tag{B.9}$$

The coadjoint action on the basis $F_i,\ i = 1, 2, 3$ is given by

$$K(g_\alpha)F = g_\alpha F g_\alpha^{-1}. \tag{B.10}$$

After finding the matrix product and writing it explicitly in the basis we find that the coordinates of the new vectors are $(0, \cos\alpha, \sin\alpha)$.

$$\begin{aligned} K(g_\alpha)(1,0,0) &= (1,0,0), \\ K(g_\alpha)(0,1,0) &= (0, \cos\alpha, \sin\alpha), \\ K(g_\alpha)(0,0,1) &= (0, -\sin\alpha, \cos\alpha). \end{aligned} \tag{B.11}$$

Therefore g_α is a rotation around x (in the zy-plane) at an angle α. We can complete the same type of calculation for the rest of the elements $g_\beta = g(0, \beta, 0)$ and $g_\gamma = g(0, 0, \gamma)$ to find out that they are indeed rotations around y- and z-axis respectively. This means that the invariant space under the transformation (B.8) is a sphere with fixed radius:

$$\Omega_r = \{F(a, b, c) = a^2 + b^2 + c^2 = r^2\}. \tag{B.12}$$

In other words the coadjoint orbits are 2-spheres parametrized by their radii.

Let us now find the natural symplectic form on the orbit $\Omega_r = S_r^2$. To do that we use equation (2.151) from chapter two to write it globally:

$$\omega_{\Omega_r, F}(K_*(X)F, K_*(Y)F) = \langle F, [X, Y]\rangle, \qquad X, Y \in \mathfrak{su}(2), F \in \mathfrak{su}(2)^*, \tag{B.13}$$

where K_* is the infinitesimal coadjoint action. The form is determined using the Killing form in the matrix space only and no additional structures are introduced on the manifold.

For practical calculations, however, it is more convenient to write the form terms of local coordinates. First let us find the expression for the coadjoint action of $\mathfrak{su}(2)$ on $\mathfrak{su}(2)^*$ in terms of the local coordinates. To do that we calculate the coadjoint action on a general element of $\mathfrak{su}(2)^*$ in local coordinates using (B.8) and (B.6) and the fact that rotations around an axis leave the basis vector associated with that axis invariant.

$$\begin{aligned} K^1(g)(a,b,c) &= a\cos\beta\cos\gamma - b\cos\beta\sin\gamma + c\sin\beta, \\ K^2(g)(a,b,c) &= a(\cos\alpha\sin\gamma - \sin\alpha\sin\beta\cos\gamma) \\ &\quad + b(\cos\alpha\cos\gamma - \sin\alpha\sin\beta\sin\gamma) - c\sin\alpha\cos\beta, \\ K^3(g)(a,b,c) &= a(\sin\alpha\sin\gamma - \cos\alpha\sin\beta\cos\gamma) \\ &\quad + b(\sin\alpha\cos\gamma + \cos\alpha\sin\beta\sin\gamma) + c\cos\alpha\cos\beta. \end{aligned} \tag{B.14}$$

Taking the derivatives at the unit element of the group allows us to find the expressions for the infinitesimal representations of the basis elements in $\mathfrak{su}(2)$ on $\mathfrak{su}(2)^*$ in terms of the coordinate basis:

$$K_*(X) = b\partial_c - c\partial_b,\ K_*(Y) = c\partial_a - a\partial_c,\ K_*(Z) = a\partial_b - b\partial_a\,. \tag{B.15}$$

Now let us find the symplectic form from equation (B.13). Using the definition for the action of a differential form on vector fields

$$(\omega_1 \wedge ... \wedge \omega_n)(X_1, ..., X_n) = \begin{vmatrix} \omega_1(X_1) & \dots & \omega_1(X_n) \\ \vdots & \ddots & \vdots \\ \omega_n(X_1) & \dots & \omega_n(X_n) \end{vmatrix}, \tag{B.16}$$

we can write a system of linear equations for the components of the symplectic form. This is done by applying the local coordinate representation of the differential form on all possible pairs constructed from (B.15).

$$\omega = \frac{a}{a^2+b^2+c^2} db \wedge dc + \frac{b}{a^2+b^2+c^2} dc \wedge da + \frac{c}{a^2+b^2+c^2} da \wedge db. \tag{B.17}$$

This is the "natural' symplectic form on the coadjoint orbit. "Natural" means that we used only the algebraic structures already existing on $SU(2)$.

To write it in a more familiar form we switch to spherical coordinates:

$$\begin{aligned} a &= r\cos\theta\cos\phi\,, \\ b &= r\cos\theta\sin\phi\,, \\ c &= r\sin\theta\,. \end{aligned} \tag{B.18}$$

Now we can write the symplectic form (B.17) in the usual way

$$\omega = r\cos\theta\, d\phi \wedge d\theta\,. \tag{B.19}$$

The form is rotationally invariant. More generally, for any group G the forms defined by (B.13) are G-invariant.