rijksuniversiteit
groningen

faculteit Wiskunde en
Natuurwetenschappen

Weyl quantization and Wigner distributions on phase space

Bachelor thesis in Physics and Mathematics

June 2014

Student: R.S. Wezeman

Supervisor in Physics: Prof. dr. D. Boer

Supervisor in Mathematics: Prof. dr H. Waalkens

Abstract

This thesis describes quantum mechanics in the phase space formulation. We introduce quantization and in particular the Weyl quantization. We study a general class of phase space distribution functions on phase space. The Wigner distribution function is one such distribution function. The Wigner distribution function in general attains negative values and thus can not be interpreted as a real probability density, as opposed to for example the Husimi distribution function. The Husimi distribution however does not yield the correct marginal distribution functions known from quantum mechanics. Properties of the Wigner and Husimi distribution function are studied to more extent. We calculate the Wigner and Husimi distribution function for the energy eigenstates of a particle trapped in a box. We then look at the semi classical limit for this example. The time evolution of Wigner functions are studied by making use of the Moyal bracket. The Moyal bracket and the Poisson bracket are compared in the classical limit. The phase space formulation of quantum mechanics has as advantage that classical concepts can be studied and compared to quantum mechanics. For certain quantum mechanical systems the time evolution of Wigner distribution functions becomes equivalent to the classical time evolution stated in the exact Egerov theorem. Another advantage of using Wigner functions is when one is interested in systems involving mixed states. A disadvantage of the phase space formulation is that for most problems it quickly loses its simplicity and becomes hard to calculate.

Keywords: Weyl quantization, phase space distributions, Wigner distribution, Moyal bracket.

Contents

1 Introduction

The begin of the 20^{th} century saw the rise of quantum mechanics. The developing quantum mechanics brought a lot of new mathematical tools with it. In quantum mechanics we talk about probabilities and expectation values of observables, one has to introduce operators acting on wave functions living in a so called Hilbert space. In quantum mechanics there does not longer exist such a thing as particle localisation. One can not know the position and momentum of a particle at the same instant in time. The idea that the mechanics is described by trajectories in phase space was completely discarded.

At that time classical mechanics was a completely developed theory defined on phase space. For this reason many people were investigating how the newly discovered quantum mechanics could be related to the the better understood classical mechanics on phase space. In 1927 Weyl [1] published a paper introducing the Weyl transform, which describes how functions acting on phase space can be related to operators acting on Hilbert space, we call this quantization. In 1932 [2] Wigner using Weyl transformations introduced the concept of how quantum mechanics can be defined on phase space. Wigner came up with distribution functions defined on phase space representing the state of the system. By averaging the Weyl transform of an observable with these so called Wigner distribution functions one could obtain the expectation value of the corresponding quantum observable. Later work independently done by both Groenewold (1946) [3] and Moyal (1949) [4] extended the theory of Wigner by introducing rules on how one should multiply phase space functions according to quantum mechanics. With this so called Moyal product one can give the time evolution of the Wigner distribution function. All combined made that quantum mechanics defined on phase space is a complete formulation of quantum mechanics and equivalent to the Hilbert operator formulation.

This thesis is devoted to the phase space formulation of quantum mechanics. It turns out that the Wigner distribution function introduced by Wigner is not the unique way of representing quantum mechanics on phase space [5][6]. We will discuss a more general class of phase space distributions. As Wigner distribution functions are the most studied and is the most applied of all phase space distributions, we will discuss them with their properties in more detail.

This outline of the thesis is as follows. We start with recalling the most important concepts of classical and quantum mechanics. In section 3 we discuss quantization and in particular the Weyl quantization which lays the basis for the Wigner distribution function. In sections 4 and 5 we introduce general phase space distributions and we take an extensive look at the Wigner and the Husimi distribution. In section 6 we explicitly calculate the Wigner distribution function for the static problem of a particle trapped in a box. In section 7 we discuss the time evolution of the Wigner distribution functions using the Moyal bracket.

2 Formalism in mechanics

In this section we will introduce the formalism and recall key concepts of classical and quantum mechanics used in this thesis. The main references for this section are [7], [8] and [9].

All physical theories consist of three parts:

I *State space:* The different possible configurations of a system are described by states. All possible states combined form the state space.

II *Observables:* These are the quantities physicists would like to measure. The spectrum is the set of all possible outcomes of a measurement.

III *Equation for time evolution:* In order to make predictions one is interested in how states and observables evolve in time. The energy functions generate the time evolution.

The dynamics will be discussed in section 7. In the whole thesis we will restrict ourselves to the one dimensional situation.

2.1 Classical mechanics

2.1.1 Classical state space

In classical mechanics the state space is called the phase space.

Definition 2.1 (Phase space)**.** *Phase space is the cotangent space of configuration space and will be denoted by $\mathcal{P}$*

$$\mathcal{P} = T^*\mathbb{R}_q \cong \mathbb{R}_q \times \mathbb{R}_p. \tag{2.1}$$

2.1.2 Classical states

At a given time t the system is determined by the position $q(t)$ and the momentum $p(t)$. Pure states are represented by a point in phase space $\mathcal{P}$.

Definition 2.2 (Classical state)**.** *A classical state is a normed probability measure μ on phase space, that is*

$$\begin{aligned} &\mu(U) \geq 0, && \textit{for all Borel sets } U \subseteq \mathcal{P}, \\ &\mu(\mathcal{P}) = 1. && \end{aligned} \tag{2.2}$$

In this context pure states are point measures.

2.1.3 Classical observables

Classical observables are given by real valued functions $f \in \mathcal{C}^\infty(\mathcal{P})$. The spectrum of an observables f is given by the image $\mathrm{Im}f$ of the corresponding function. Lastly the expectation value of a classical observables in a given state μ is calculated by

$$\langle f \rangle = \int f(q,p)\mathrm{d}\mu(q,p), \tag{2.3}$$

where the integration is over the whole phase space $\mathcal{P}$. In the rest of the thesis we will omit writing the limits of integrals which are over all space, whether that be phase space or Hilbert space.

2.2 Quantum mechanics

Quantum mechanics has the property that it is restricted by the uncertainty relation given by

$$\Delta x \Delta p \geq \frac{1}{2}\hbar. \tag{2.4}$$

One cannot measure the position and momentum simultaneously up to arbitrary precision. Due to this we no longer have phase space as state space.

2.2.1 Quantum state space

In quantum mechanics the state space is a Hilbert space.

Definition 2.3 (Hilbert space)**.** *Hilbert space denoted by $\mathcal{H}$ is a complete inner product space, with complex inner product denoted by $\langle \cdot, \cdot \rangle$.*

$$\mathcal{H} = L^2(\mathbb{R}) := \{\phi : \mathbb{R} \to \mathbb{C} | \int |\phi(q)|^2 \, \mathrm{d}q < \infty\}, \tag{2.5}$$

and the inner product defined by

$$\langle \phi, \psi \rangle := \int \phi(q)^* \psi(q) \mathrm{d}q. \tag{2.6}$$

We will make use of Dirac notation, vectors in Hilbert space are denoted by the kets $|\alpha\rangle$. For each vector $|\alpha\rangle$ in Hilbert space $\mathcal{H}$ we have a vector in the dual space $\mathcal{H}^*$ denoted by a bra $\langle\alpha|$ according to proposition 2.1.

Proposition 2.1 (Co-vector)**.** *Let $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ denote a Hilbert space and let $|\alpha\rangle \in \mathcal{H}$ be a vector. Then*

$$|\alpha\rangle \to \langle |\alpha\rangle, - \rangle = \langle \alpha| ,$$

is a linear isomorphism from $\mathcal{H} \to \mathcal{H}^*$.

The proof follows directly from properties of the inner product. We can now denote the complex inner product between two vectors in Hilbert space as $\langle \alpha | \beta \rangle$.

For complex inner products we have the Cauchy-Schwarz inequality [7],

$$|\langle \psi | \phi \rangle|^2 \leq \langle \psi | \psi \rangle \langle \phi | \phi \rangle . \tag{2.7}$$

A basis $\{|\phi_i\rangle\}$ is a set of linearly independent vectors in a finite Hilbert space such that every vector $|\psi\rangle$ can be written as a linear combination of basis vectors

$$|\psi\rangle = \sum_i a_i |\phi_i\rangle .$$

Definition 2.4. *The basis $\{|\phi_i\rangle\}$ is called orthonormal if it satisfies*

$$\langle \phi_i | \phi_j \rangle = \delta_{ij}. \tag{2.8}$$

2.2.2 Quantum operators and observables

Definition 2.5 (Operator)**.** *In quantum mechanics an operator $\hat{A}$ is a linear mapping between two vectors in Hilbert space given by*

$$\hat{A} : \mathcal{D}(\hat{A}) \subseteq \mathcal{H} \to \mathcal{H}. \tag{2.9}$$

Here $\mathcal{D}(\hat{A})$ is the domain of the operator $\hat{A}$.

All observables in quantum mechanics are represented by hermitian operator.

The expectation value of an observable $\hat{A}$ for a given normalized state $|\Psi\rangle$ is given by

$$\langle \hat{A} \rangle = \langle \Psi | \hat{A} \Psi \rangle . \tag{2.10}$$

In quantum mechanics one measures expectation values. The spectrum of an operator $\hat{A}$ is given by all the values $\langle A \rangle \in \mathbb{R}$ can attain, denoted by $\sigma(\hat{A})$.

Definition 2.6 (Outer product)**.** *The outer product between two vectors $|\alpha\rangle$ and $|\beta\rangle \in \mathcal{H}$ is defined as*

$$|\beta\rangle \langle \alpha| . \tag{2.11}$$

It can easily be seen that the outer product is a linear operator. When acting on a vector in Hilbert space it gives back a new vector in Hilbert space.

Definition 2.7 (Projection operator)**.** *The projection operator of a normalized vector $|\alpha\rangle$ is defined as*

$$\hat{P} = |\alpha\rangle \langle\alpha| . \tag{2.12}$$

For an orthonormal continuous basis $\{|\phi_z\rangle\}$ we have the continuous orthonormality version of (2.8).

$$\langle\phi_z|\phi_{z'}\rangle = \delta(z - z'). \tag{2.13}$$

An important property of the projection operator is that for a complete continuous basis $\{|\phi_z\rangle\}$ it satisfies

$$\int |\phi_z\rangle \langle\phi_z| \, \mathrm{d}z = \hat{\mathbb{1}}, \tag{2.14}$$

where $\hat{\mathbb{1}}$ is the identity operator in $\mathcal{H}$.

2.2.3 Quantum states

In quantum mechanics pure states are represented by normalized vectors $|\psi\rangle \in \mathcal{H}$. A statistical ensemble of pure states is a mixed state. Mixed states cannot be described by a vector. For the normalized pure state $|\psi\rangle$ one can look at the orthogonal projection

$$\hat{P}_\psi = |\psi\rangle \langle\psi| . \tag{2.15}$$

For the generalization of pure states we introduce the density operator $\hat{\rho}$. The density operator is defined with the use of the trace.

Definition 2.8 (Trace)**.** *The trace of an operator $\hat{A}$ is the sum of all diagonal elements given by,*

$$\mathrm{Tr}[\hat{A}] = \int \langle\phi_z| \hat{A} |\phi_z\rangle \, \mathrm{d}z, \tag{2.16}$$

where the set $\{|\phi_z\rangle\}$ is a complete continuous orthonormal basis of $\mathcal{H}$.

A well known property of the trace is that it is independent of the choice of basis. The above defined pure state $\hat{P}_\psi$ has trace 1 which can be seen by direct substitution. Another direct property of the definition of $\hat{P}_\psi$ is that

$$\langle\phi|\hat{P}_\psi|\phi\rangle \geq 0, \qquad \forall \phi \in \mathcal{H}. \tag{2.17}$$

Definition 2.9 (Quantum state)**.** *The quantum state or the density operator $\hat{\rho}$ is a positive hermitian operator with trace 1 i.e. [8]*

$$\langle\phi| \hat{\rho} |\phi\rangle \geq 0, \qquad \forall \phi \in \mathcal{H}, \tag{2.18a}$$

$$\hat{\rho}^\dagger = \hat{\rho}, \tag{2.18b}$$

$$\mathrm{Tr}[\hat{\rho}] = 1. \tag{2.18c}$$

For pure states the density operator has the form

$$\hat{\rho} = |\Psi\rangle \langle\Psi| . \tag{2.19}$$

Due to the fact that $|\Psi\rangle$ is normalized for a pure state the density operator has the property

$$\hat{\rho} = \hat{\rho}^2. \tag{2.20}$$

This means that for a pure state the density operator is an orthogonal projection operator. However for mixed states this equality does not hold. In fact this result can be used to determine whether a state is a pure or a mixed state [8]

$$0 < \mathrm{Tr}[\hat{\rho}^2] \leq 1. \tag{2.21}$$

The equality in equation (2.21) holds if and only if $\hat{\rho}$ is a pure state.

The general density operator $\hat{\rho}$ for a mixed state can be expanded in terms of orthogonal pure states according to

$$\hat{\rho} = \sum_i P_i \left|\Psi_i\right\rangle \left\langle\Psi_i\right|, \tag{2.22}$$

where for normalization we have that P_i satisfy

$$\begin{aligned} &0 \leq P_i \leq 1, \qquad\qquad i \geq 2, \\ &\textstyle\sum_i P_i = 1. \end{aligned} \tag{2.23a}$$

The P_i have a probability interpretation. Mixed states can be represented in infinitely many different ways by choosing a different basis of pure states. Mixed states have the property that they can not be represented as just one ket vector.

Definition 2.10 (Expectation value)**.** *The expectation value of an operator* $\hat{A}$ *is given by* $\mathrm{Tr}[\hat{A}\hat{\rho}]$

This definition agrees with equation (2.10) when $\hat{\rho}$ is a pure state.

$$\begin{aligned} \langle A\rangle &= \langle\Psi|\hat{A}|\Psi\rangle \\ &= \int \langle\Psi|\phi_z\rangle \langle\phi_z|\hat{A}|\Psi\rangle \,\mathrm{d}z \\ &= \int \langle\phi_z|\hat{A}|\Psi\rangle \langle\Psi|\phi_z\rangle \,\mathrm{d}z \\ &= \mathrm{Tr}[\hat{A}\hat{\rho}]. \end{aligned} \tag{2.24}$$

Here we used in the second step that for an orthogonal basis $\{|\phi_z\rangle\}$ the projection operator is the identity. In the third step we commuted the scalars which concludes the proof.

The section is summarized in the following table 1 from [9]

	Classical	*Quantum*
Observables	$f \in C^\infty(\mathbb{R}^d_x \times \mathbb{R}^d_p, \mathbb{R})$	selfadjoint operators acting on Hilbert space $L^2(\mathbb{R}^d)$
Building block observables	position x and momentum p	position $\hat{x}$ and momentum $\hat{p}$ operators
Possible results of measurements	$\mathrm{im}(f)$	$\sigma(\hat{A})$
States	probability measures μ on phase space $\mathbb{R}^d_x \times \mathbb{R}^d_p$	density operators $\hat{\rho}$ on $L^2(\mathbb{R}^d)$
Pure states	points in phase space $\mathbb{R}^d_x \times \mathbb{R}^d_p$	wave functions $\psi \in L^2(\mathbb{R}^d)$

Table 1: Comparison of classical mechanics with quantum mechanics [9].

We end this section by giving the frequently used Campbell-Baker-Hausdorff identity [8]

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}, \qquad\qquad \text{if } [A,[A,B]] = [B,[A,B]] = 0. \tag{2.25}$$

For the cannonical operators $\hat{q}$ and $\hat{p}$ we have the commutation relation given by

$$[\hat{q}, \hat{p}] = i\hbar. \tag{2.26}$$

If we now use the Campbell-Baker-Hausdorff identity on these operators we find

$$e^{i\xi\hat{q}+i\eta\hat{p}} = e^{i\xi\hat{q}}e^{i\eta\hat{p}}e^{i\frac{\hbar}{2}\xi\eta}. \tag{2.27}$$

2.3 Coherent states

When describing the quantum states of the radiation field it can be convenient to consider the so called coherent (α) state space rather than the usual (q, p) phase space. In this section we will shorty introduce coherent states as done in [10]. The radiation field can be described by the modes of the harmonic oscillator. Recall the solution of the harmonic oscillator which can be found in many standard quantum mechanics books for example [7] [8] [11]. For the harmonic oscillator with mass m and frequency ω we introduce the annihilation and creation operators given by

$$\hat{a} = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{q} + i\hat{p}), \tag{2.28}$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{q} - i\hat{p}). \tag{2.29}$$

We can also express the position and momentum operator in terms of the annihilation and creation operators

$$\hat{q} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger), \tag{2.30}$$

$$\hat{p} = \sqrt{\frac{\hbar m\omega}{2}}(\hat{a} - \hat{a}^\dagger). \tag{2.31}$$

The annihilation and creation operators have the following properties

$$[\hat{a}, \hat{a}^\dagger] = \hat{\mathbb{1}}, \tag{2.32a}$$

$$\hat{a}\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle, \tag{2.32b}$$

$$\hat{a}^\dagger\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle, \tag{2.32c}$$

$$\hat{a}\left|0\right\rangle = 0. \tag{2.32d}$$

Here $|n\rangle$ denotes the n^{th} eigenstate of the harmonic oscillator with as ground state $|0\rangle$.

Definition 2.11 (Displacement operator in coherent state space)**.** *For a complex number α the displacement operator is the unitary operator $\hat{D}(\alpha)$ given by*

$$\hat{D}(\alpha) = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}. \tag{2.33}$$

We can rewrite the displacement operator as

$$\begin{aligned}\hat{D}(\alpha) &= e^{\mathrm{Re}(\alpha)(\hat{a}^\dagger - \hat{a}) + i\mathrm{Im}(\alpha)(\hat{a}^\dagger + \hat{a})} \\ &= e^{\frac{i}{\hbar}(p_0\hat{x} - q_0\hat{p})} \\ &= D(q_0, p_0),\end{aligned} \tag{2.34}$$

where $D(q_0, p_0)$ is the displacement operator on the phase space with q_0 and p_0 given by

$$q_0 = \sqrt{\frac{2\hbar}{m\omega}}\mathrm{Re}(\alpha), \tag{2.35}$$

$$p_0 = \sqrt{2\hbar m\omega}\,\mathrm{Im}(\alpha). \tag{2.36}$$

Thus the point α is related to the point (q_0, p_0) in phase space by

$$\alpha = \sqrt{\frac{m\omega}{2\hbar}} q_0 + i \frac{1}{\sqrt{2\hbar m\omega}} p_0. \tag{2.37}$$

Definition 2.12 (Coherent state)**.** *For the complex number α the coherent state $|\alpha\rangle$ is defined by*

$$|\alpha\rangle = \hat{D}(\alpha) |0\rangle. \tag{2.38}$$

Straightforward calculation using properties (2.32) yields a more explicit form of the coherent state

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \tag{2.39}$$

The coherent state has the property that it is an eigenstate of the annihilation operator with eigenvalue α.

The set of coherent states is an overcomplete basis *i.e.*

$$\frac{1}{\pi} \int \mathrm{d}^2\alpha \, |\alpha\rangle \langle\alpha| = \hat{\mathbb{1}}, \tag{2.40}$$

where $\mathrm{d}^2\alpha = \mathrm{dRe}(\alpha)\mathrm{dIm}(\alpha)$.

The uncertainty in position and momentum of the coherent state is given by

$$\Delta q = \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar}{m\omega}}, \tag{2.41}$$

$$\Delta p = \frac{1}{\sqrt{2}} \sqrt{\hbar m\omega}, \tag{2.42}$$

which means that the coherent states satisfy the minimum uncertainty limit given by

$$\Delta q \Delta p = \frac{\hbar}{2}. \tag{2.43}$$

A squeezed coherent state is a minimum uncertainty state but with a different ratio in the uncertainty of position and momentum compared to the coherent state.

3 Quantization

A quantization is a rule how to assign operators acting on Hilbert space to functions defined on the phase space. Dirac came up with the following quantization for position and momentum [9]. Assign to the position variable q the operator $\hat{q}$ and to the momentum variable p the operator $\hat{p}$ according to

$$(\hat{q}\phi)(q) := q\phi(q), \qquad \phi \in L^2(\mathbb{R}), \tag{3.1}$$

$$(\hat{p}\phi)(q) := -i\hbar\partial_q\phi(q), \qquad \phi \in L^2(\mathbb{R}) \cap \mathcal{C}^1(\mathbb{R}). \tag{3.2}$$

We call the function A corresponding to the operator $\hat{A}$ the symbol of $\hat{A}$. Dirac's quantization rules only gives a complete description for functions which are linear in q and p. The problem arises once one tries to quantize functions such as $q \cdot p$. Because q and p do commute with respect to the standard multiplication there are many different possibilities, for example one could quantize $q \cdot p$ as

$$\begin{array}{ccc} \hat{q}\cdot\hat{p}, & \hat{p}\cdot\hat{q} = \hat{q}\cdot\hat{p} - i\hbar\hat{\mathbb{1}}, & \frac{1}{2}(\hat{q}\cdot\hat{p} + \hat{p}\cdot\hat{q}). \\ Standard-ordered & Antistandard-ordered & Symmetric-ordered \end{array} \tag{3.3}$$

These three possible quantization rules for qp are all different operators due the fact that $\hat{q}$ and $\hat{p}$ do not commute but have as commutation relation (2.26). We call the ordering standard-ordered if we place all $\hat{q}$ in front. Similar if we place $\hat{p}$ in front we call the ordering anti standard-ordered. The third example is a symmetric-ordered operator. The to be discussed Weyl quantization, assigns to $q \cdot p$ exactly this last symmetric-ordered operator.

One needs to specify how to treat different ordering to give a full prescription for functions which are non linear in q and p.

Definition 3.1 (Quantization)**.** *A quantization of a classical system is a linear map $\mathcal{Q}$ from the functions $f \in \mathcal{C}^\infty(\mathcal{P})$ into operators $\mathcal{Q}(f)$ acting on $\mathcal{H}$ satisfying Dirac's conditions* (3.1),(3.2) *and [12]*

$$\mathcal{Q}(1) = \hat{\mathbb{1}}, \tag{3.4a}$$

$$\mathcal{Q}(\overline{f}) = \mathcal{Q}(f)^*. \tag{3.4b}$$

Once we applied a quantization we want to define a product $\sharp_\hbar$ on the phase functions such that

$$\widehat{f(q,p)\sharp_\hbar g}(q,p) = \hat{f}\hat{g}. \tag{3.5}$$

Here the hat denotes the quantized function and on the right hand side we have the usual operator product. Different rules for quantization give rise to different phase space products $\sharp_\hbar$. This product must agree with the non-commutativity of the operator product. We thus also require $q\sharp_\hbar p$ to approximate when $\hbar \to 0$ to the normal product $q \cdot p$. This is due to the fact that for small $\hbar$ the commutation relation (2.26) becomes small and the operators start to approximately commute.

3.1 Weyl quantization

Weyl quantization leaves the quantization of Dirac given by (3.1) and (3.2) intact. Additionally we now give a more general prescription for how to treat function of (q, p) by making use of the Weyl transform. The Weyl transform is a one-to-one function Φ it assigns to functions on the phase space a corresponding operator in Hilbert space. Before we introduce the Weyl transform we first need to introduce a two concepts.

Definition 3.2 (Schwartz space)**.** *The space of Schwartz functions on the phase space is given by [9]*

$$\mathcal{S}(\mathcal{P}) = \left\{ f \in \mathcal{C}^\infty(\mathcal{P}) | \forall a, \alpha \in \mathbb{N}_0 : \|f\|_{a,\alpha} < \infty \right\}. \tag{3.6}$$

In the above definition the semi norm is given by

$$\|f\|_{a,\alpha} := \sup_{x\in\mathcal{P}} \left| x^a \partial_x^\alpha f(x) \right|. \tag{3.7}$$

Definition 3.3 (Bounded operator)**.** *Let $\mathcal{X}$ and $\mathcal{Y}$ be normed spaces. The linear operator $\hat{A} : \mathcal{X} \to \mathcal{Y}$ is called bounded if $\exists M \geq 0$ such that $\forall x \in \mathcal{X}$ we have that [9]*

$$\|\hat{A}x\|_{\mathcal{Y}} \leq M\|x\|_{\mathcal{X}}. \tag{3.8}$$

The space of all linear bounded operators between $\mathcal{X}$ and $\mathcal{Y}$ is denoted by $\mathcal{B}(\mathcal{X}, \mathcal{Y})$. If the operators maps $\mathcal{X}$ to itself we will simply denote the space of bounded operators by $\mathcal{B}(\mathcal{X})$.

Definition 3.4 (Weyl transform)**.** *The Weyl transform is the function Φ which maps functions $A \in \mathcal{S}(\mathcal{P})$ one-to-one to the operator $\hat{A} \in \mathcal{B}(\mathcal{H})$ according to[13]*

$$\hat{A} = \Phi[A] = \left(\frac{1}{2\hbar\pi}\right)^2 \iiiint A(q,p) e^{\frac{i}{\hbar}(\xi(\hat{q}-q)+\eta(\hat{p}-p))} \mathrm{d}q\mathrm{d}p\mathrm{d}\xi\mathrm{d}\eta. \tag{3.9}$$

As the mapping is one-to-one the inverse exists and is given by [14]

$$A(q,p) = \Phi^{-1}[\hat{A}](q,p) = \int e^{-i\frac{py}{\hbar}} \langle q + \frac{y}{2} |\, \hat{A} \,| q - \frac{y}{2} \rangle \, \mathrm{d}y. \tag{3.10}$$

Here A is the (Weyl) symbol of the operator $\hat{A}$.

The phase space product related to the Weyl transform is denote by $\star_M$. The product $\star_M$ is called the Moyal product however was first introduced by Groenewold in 1946 [3]. It satisfies condition (3.5)

$$\Phi[A(q,p) \star_M B(q,p)] = \Phi[A(q,p)] \cdot \Phi[B(q,p)]. \tag{3.11}$$

The Moyal product is the operation $\mathcal{S}(\mathcal{P}) \times \mathcal{S}(\mathcal{P}) \to \mathcal{S}(\mathcal{P})$ such that (3.11) is satisfied, and it can be represented by [13]

$$A(q,p) \star_M B(q,p) = A(q,p) \exp\left(i\frac{\hbar}{2}(\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q}) \right) B(q,p). \tag{3.12}$$

Here the arrows indicate whether the partial differentiation acts to the left or to the right. It can easily be seen that $\star_M$ is not commutative, which follows directly from the fact that the normal operator product in Hilbert space is not commutative. The Moyal product however is an associative operation which follows directly from inspection of the formula (3.11). The Moyal product is used in the definition of the Moyal bracket.

Definition 3.5 (Moyal bracket)**.** *The Moyal bracket is a bilinear operation $\mathcal{C}^\infty(\mathcal{P}) \times \mathcal{C}^\infty(\mathcal{P}) \to \mathbb{C}$ given by*

$$\{A(q,p), B(q,p)\}_M = \frac{1}{i\hbar} \left(A(q,p) \star_M B(q,p) - B(q,p) \star_M A(q,p) \right). \tag{3.13}$$

The explicit form of the Moyal product and Moyal bracket will be derived in appendix A and further discussed in section 7.

4 Quantum mechanics in phase space

In classical mechanics the states are described by normed probability measures. This means that we deal with a joint probability density $\rho_C(q,p)$ over phase space describing the state of the system. This joint probability density has the properties that it is normalised and is positive [15]. If we take the marginals of $\rho_C(q,p)$ we find the probability densities in position or momentum space. If we want to describe quantum mechanics similar to classical mechanics we need a quantum joint 'probability' density.

Suppose that for a given state $\hat{\rho}$ there exist a similar density function $\rho_Q(q,p)$ over phase space. This function $\rho_Q(q,p)$ should satisfy a few properties. First of all if we take the marginals of this function we would like to get back our well known probability density in momentum and position space.

$$\int \mathrm{d}p \rho_Q(q,p) = \langle q| \hat{\rho} |q\rangle , \tag{4.1a}$$

$$\int \mathrm{d}q \rho_Q(q,p) = \langle p| \hat{\rho} |p\rangle . \tag{4.1b}$$

If we want to interprete $\rho_Q(q,p)$ as an joint probability density we also require

$$\rho_Q(q,p) \geq 0 \qquad \forall (q,p) \in \mathcal{P}. \tag{4.2}$$

It appears that there exist many different non equivalent functions $\rho_Q(q,p)$ satisfying (4.1) and (4.2) [5]. By imposing additional physical restrictions on $\rho_Q(q,p)$ one can come up with a more restricted set of distributions. Recall for mixed states, $\hat{\rho}$ can be expressed in infinitely many different ways by choosing different basis sets $\{\psi_i\}$.

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle \langle\psi_i| . \tag{4.3}$$

If we now additionally require $\rho_Q(q,p)$ to be independent of the choice of basis for $\hat{\rho}$, which is a fair restriction in the sense that the mechanics should not change for different choice basis. We will call this the *mixture property*. The mixture property is a generalisation of requiring the density functions to be bilinear in the wave function. Then it turns out that due to this restriction we no longer can satisfy condition (4.1) both with (4.2) proven by Wigner [16] and generalized by Srinivas [17]. It appears we need to make a choice which condition we value more. The Wigner function satisfies the mixture property and (4.1) but not (4.2). The Wigner function thus can not be interpreted as a probability distribution as it can attain negative values. The Husimi distribution does satisfy the nonnegative condition but does not satisfy (4.1).

4.1 General form

There are still infinitely many different probability densities which satisfy the mixture property listed above. Once we found a satisfying probability density ρ we would like to calculate expectation values of observables. With the interpretation of ρ being a probability density we calculate the expectation value of an operator $\hat{A}$ according to

$$\mathrm{Tr}[\hat{\rho}(\hat{q},\hat{p},t)\hat{A}(\hat{q},\hat{p})] = \iint A(q,p)\rho(q,p,t)\mathrm{d}p\mathrm{d}q. \tag{4.4}$$

Here we naively use that the scalar function $A(q,p)$ is related to $\hat{A}(\hat{q},\hat{p})$ by simply replacing the operators $(\hat{q},\hat{p})$ by the scalars correspondence (q,p) given by (3.1) and (3.2).

It follows immediately that this does not specify a unique probability distribution ρ, which can be seen by the following illustrative example.

Example 4.1 (non uniqueness of ρ)**.** Consider calculating the expectation value of the operator $\hat{A}(\hat{q},\hat{p}) = e^{i\xi\hat{q}+i\eta\hat{p}}$ where ξ and η are arbitrary constants. By equation (4.4) we find,

$$\mathrm{Tr}[\hat{\rho}(\hat{q},\hat{p},t)e^{i\xi\hat{q}+i\eta\hat{p}}] = \iint e^{i\xi q+i\eta p}\rho^a(q,p,t)\mathrm{d}p\mathrm{d}q. \tag{4.5}$$

Similarly we can calculate the expectation value of a different operator $\hat{B}(\hat{q},\hat{p}) = e^{i\xi\hat{q}}e^{i\eta\hat{p}}$ given by,

$$\mathrm{Tr}[\hat{\rho}(\hat{q},\hat{p},t)e^{i\xi\hat{q}}e^{i\eta\hat{p}}] = \iint e^{i\xi q+i\eta p}\rho^b(q,p,t)\mathrm{d}p\mathrm{d}q. \tag{4.6}$$

The two operators are related by (2.27)

$$\hat{A} = \hat{B}e^{i\frac{\hbar}{2}\xi\eta}. \tag{4.7}$$

These operators are certainly different. From this we conclude that in general the expectation values must also be different. However by transforming $\hat{B}(\hat{q},\hat{p})$ into a scalar function $B(q,p)$ the exponents start to commute. In the case $\rho^a = \rho^b$ the right hand sides of (4.5) and (4.6) become equal. But this cannot be as the expectation values for $\hat{A}$ and $\hat{B}$ might differ, from which we conclude $\rho^a \neq \rho^b$.

We learn from this example that we need to specify how we associate an operator to a function in phase space. In the first example above for the equation (4.5) the operator and function were associated according to

$$e^{i\xi\hat{q}+i\eta\hat{p}} \longleftrightarrow e^{i\xi q+i\eta p}.$$

We used a different association rule for the second example in equation (4.6) namely,

$$e^{i\xi\hat{q}+i\eta\hat{p}}e^{-i\frac{\hbar}{2}\xi\eta} \longleftrightarrow e^{i\xi q+i\eta p}.$$

Both these association rules generate non equivalent phase space densities ρ. From this Lee [6] deduced a general class of phase space distributions given by

$$\mathrm{Tr}[\hat{\rho}(\hat{q},\hat{p},t)e^{i\xi\hat{q}+i\eta\hat{p}}f(\xi,\eta)] = \iint e^{i\xi q+i\eta p}\rho^f(q,p,t)\mathrm{d}p\mathrm{d}q. \tag{4.8}$$

In this equation $f(\xi,\eta)$ is a function of ξ and η such that it specifies different association rules. Different densities are now denoted by $\rho^f(q,p)$ as they do depend on different choices for $f(\xi,\eta)$.

Using a Fourier transform we can rewrite equation (4.8) into a formula for $\rho^f(q,p)$ given by

$$\rho^f(q,p) = \frac{1}{4\pi^2}\iiint \mathrm{d}\eta\mathrm{d}q'\mathrm{d}p\,\langle q' + \frac{1}{2}\eta\hbar|\hat{\rho}|q' - \frac{1}{2}\eta\hbar\rangle\, f(\xi,\eta)e^{i\xi(q'-q)-i\eta p}. \tag{4.9}$$

With the result of equation (4.8) we can now generate different phase space distributions by deciding a rule for assigning operators to their corresponding function in phase space. The most common way of assigning an operator to its corresponding function is by bringing the operator in some ordering. The most common orderings are standard-ordered, anti standard-ordered, normal-ordered, anti normal-ordered and the in previous section discussed Weyl quantisation.

When a system is described in terms of annihilation and creation operators the system is in normal-ordered when all creation operators are to the left of all annihilation operators in the product. A system is in anti normal-ordered form when all annihilation operators are to the left of all creation operators illustrated in the following example.

Example 4.2 (Anti- and normal-ordered operator)**.** We can bring the operator $\hat{A}$ given by

$$\hat{A} = e^{\hat{a}+\hat{a}^\dagger}, \tag{4.10}$$

in normal-ordered form $:\hat{A}:$ given by

$$:\hat{A}:= e^{\hat{a}^\dagger}e^{\hat{a}}, \tag{4.11}$$

and in anti normal-ordered form $;\hat{A};$ given by

$$;\hat{A};= e^{\hat{a}}e^{\hat{a}^\dagger}. \tag{4.12}$$

Lee discusses in his article all these different orderings with their corresponding distribution functions [6]. We summarize his findings in table 2 and 3.

Distribution function	Rules of association	f
Wigner d.f. function (ρ^W)	$e^{i\xi q+i\eta p} \leftrightarrow e^{i\xi\hat{q}+i\eta\hat{p}}$	1
Standard-ordered d.f. (ρ^S)	$e^{i\xi q+i\eta p} \leftrightarrow e^{i\xi\hat{q}}e^{i\eta\hat{p}}$	$e^{-i\frac{\hbar}{2}\xi\eta}$
Anti standard-ordered (Q-) d.f. (ρ^{AS})	$e^{i\xi q+i\eta p} \leftrightarrow e^{i\eta\hat{p}}e^{i\xi\hat{q}}$	$e^{+i\frac{\hbar}{2}\xi\eta}$
Normal-ordered (P-) d.f. (ρ^N)	$e^{i\xi q+i\eta p} = e^{z\alpha^*-z^*\alpha} \leftrightarrow e^{z\hat{a}^\dagger}e^{-z^*\hat{a}}$	$e^{\frac{\hbar\xi^2}{4m\omega}+\frac{\hbar m\omega\eta^2}{4}} = e^{\frac{1}{2}\lvert z\rvert^2}$
Anti normal-ordered d.f. (ρ^{AN})	$e^{i\xi q+i\eta p} = e^{z\alpha^*-z^*\alpha} \leftrightarrow e^{-z^*\hat{a}}e^{z\hat{a}^\dagger}$	$e^{-\frac{\hbar\xi^2}{4m\omega}-\frac{\hbar m\omega\eta^2}{4}} = e^{-\frac{1}{2}\lvert z\rvert^2}$
Generalized anti normal ordered d.f. (ρ^H) (Husimi d.f.)	$e^{i\xi q+i\eta p} = e^{\nu\beta^*-\nu^*\beta} \leftrightarrow e^{-\nu^*\hat{b}}e^{\nu\hat{b}^\dagger}$	$e^{-\frac{\hbar\xi^2}{4m\kappa}-\frac{\hbar m\kappa\eta^2}{4}} = e^{-\frac{1}{2}\lvert\nu\rvert^2}$

Table 2: Different types of distribution functions (d.f.) with their corresponding rule of association and function f [6]

In table 2 the normal and anti normal ordered distribution functions are with respect to the annihilation and creation operators associated to the harmonic oscillator given by (2.28).

In the table used α is given by (2.37) and z is given by,

$$z = i\xi\sqrt{\frac{\hbar}{2m\omega}} - \eta\sqrt{\frac{\hbar m\omega}{2}}. \tag{4.13}$$

The normal-ordered distribution function is also often called the P-distribution where the anti normal-ordered distribution is named the Q-distribution function.

The Husimi distribution is a generalisation of the anti normal ordered equation. The generalized operator $\hat{b}$ is found by replacing ω with κ in equations (2.28). A similar equation holds ν by replacing ω with κ in equation (4.13). The Q-distribution can be defined using coherent states where the Husimi distribution is the generalization using squeezed coherent states. This is discussed in more detail in section 5.

We now list some of the properties given by Lee [6].

d.f.	Properties			
	a) Bilinear	b) Real	c) Nonnegative	d) marginal distributions
Wigner (ρ^W)	yes	yes	no	yes
Standard (ρ^S)	yes	no	no	yes
Anti standard (ρ^{AS})	yes	no	no	yes
Normal (ρ^N)	yes	yes	no	no
Anti normal (ρ^{AN})	yes	yes	yes	no
Husimi (ρ^H)	yes	yes	yes	no

Table 3: Properties of the listed distribution functions [6]

The properties are explained

a) Bilinear, the distribution is bilinear in the wave function Ψ. For general distribution functions we map from $\mathcal{H} \times \mathcal{H}$ to a phase space distribution function $\rho_Q(q,p)$, we require this mapping to be bilinear. An example of a bilinear mapping is the outer product between two pure states given by (2.11). The density operator is an outer product and thus is an allowed bilinear form. The fact that this bilinear condition is satisfied for all of the above distribution functions is a direct result of $f(\xi, \eta)$ being independent of Ψ and $\hat{\rho}$ being a bilinear form of the wave function.

b) Real, the distribution only takes real values.

c) Nonnegative, the distribution does not attain negative values on the whole domain.

d) Marginal distributions, the distribution satisfy correct marginals given by the equations (4.1).

According to table 3 all the listed distribution functions are bilinear. O'Connel and Wigner proved that there does not exist a quantum phase space distribution which is bilinear, satisfies the marginal distributions and is nonnegative [16]. Thus none of these distribution functions satisfy all properties of a classical joint probability distribution. We call these distribution functions for this reason quasiprobability distribution functions.

Another observation of Lee's results is that the restriction for a distribution function to yield the correct marginal probabilities does not determine the distribution function uniquely. All these distribution functions are in a sense equivalent as they all can yield the correct expectation value for observables.

In the rest of this thesis we will focus on the Wigner and the Husimi distribution function. The reason we focus on these two distributions is because they are the most studied and most applied distribution functions. When describing the dynamics of distribution functions it is convenient to work with the Wigner function as the equations describing the dynamics of the other distribution functions become rather difficult. The Husimi distribution will be studied due to its non negative property.

4.2 Wigner function

We introduce the Wigner function ρ_W with the help of inverse Weyl transformations.

Definition 4.1 (Inverse Weyl transform). *The inverse Weyl transform is a mapping from an operator $\hat{A}$ on a Hilbert space to a function $A_w(q,p)$ on phase space defined by,*

$$A_w(q,p) = \int e^{-i\frac{py}{\hbar}} \langle q + \frac{y}{2}| \hat{A} |q - \frac{y}{2}\rangle \, \mathrm{d}y. \tag{4.14}$$

In this definition we expressed the operator $\hat{A}$ in position basis $\langle q| \hat{A} |q'\rangle$. We can also express the operator $\hat{A}$ in momentum basis which results in an equivalent expression for $A_w(q,p)$.

$$A_w(q,p) = \int e^{i\frac{qu}{\hbar}} \langle p + \frac{u}{2}| \hat{A} |p - \frac{u}{2}\rangle \, \mathrm{d}u. \tag{4.15}$$

Definition 4.2 (Wigner function). *The Wigner function for the state $\hat{\rho}$ is defined as,*

$$\rho_W(q,p) = \frac{1}{2\pi\hbar}\rho_w(q,p). \tag{4.16}$$

In this definition $\rho_w(q,p)$ is the inverse Weyl transform of the state operator $\hat{\rho}$.

Claim. *The Wigner function $\rho_W(q,p)$ satisfies the correct marginals conditions* (4.1)*.*

Proof. We prove the claim by straightforward integration of (4.15).

$$\begin{aligned}\int \rho_W(q,p)\mathrm{d}p &= \frac{1}{2\pi\hbar}\iint e^{-i\frac{py}{\hbar}} \langle q + \frac{y}{2}| \hat{\rho} |q - \frac{y}{2}\rangle \, \mathrm{d}y\mathrm{d}p \\ &= \frac{1}{2\pi\hbar}\int 2\pi\hbar\delta(y) \langle q + \frac{y}{2}| \hat{\rho} |q - \frac{y}{2}\rangle \, \mathrm{d}y,\end{aligned} \tag{4.17}$$

where we integrated over the p variable and we made use of

$$\int e^{-i\frac{py}{\hbar}}\mathrm{d}p = 2\pi\hbar\delta(y). \tag{4.18}$$

If we now integrate this with respect to y we find the desired result (4.1a).

$$\int \rho_W(q,p)\mathrm{d}p = \langle q|\,\hat{\rho}\,|q\rangle\,. \tag{4.19}$$

A similar integration over position space of $\rho_W(q,p)$ expressed in the momentum basis yields (4.1b). □

This property of the Wigner function satisfying the correct marginal probabilities is a well known property of joint probability distributions. However as stated before the Wigner function in general attains negative values and thus can not be interpreted as a real probability distribution function. We will look at a few more properties of the Wigner function.

First of all we required for the distribution functions to be bilinear in the wave function.

Claim. *The Wigner function is bilinear in the wave function.*

Proof. This is a direct consequence of the form of the Wigner distribution function. As $\hat{\rho}$ is in a bilinear form the Wigner function is bilinear in the wave function. □

Claim. *The Wigner function is real valued.*

Proof. It is sufficient to show that $\rho_w(q,p)$ is a real valued function.

$$\rho_w(q,p)^* = \int e^{+i\frac{py}{\hbar}}\,\langle q-\frac{y}{2}|\,\hat{\rho}^\dagger\,|q+\frac{y}{2}\rangle\,\mathrm{d}y. \tag{4.20}$$

Making use of $\hat{\rho}^\dagger = \hat{\rho}$ and a change of variables from $y = -y'$ we find that,

$$\begin{aligned}\rho_w(q,p)^* &= \int e^{-i\frac{py'}{\hbar}}\,\langle q+\frac{y}{2}|\,\hat{\rho}\,|q-\frac{y}{2}\rangle\,\mathrm{d}y' \\ &= \rho_w(q,p).\end{aligned} \tag{4.21}$$

□

Claim. *The Wigner function is normalized.*

Proof.

$$\begin{aligned}\iint \rho_W(q,p)\mathrm{d}q\mathrm{d}p &= \int \langle q|\,\hat{\rho}\,|q\rangle\,\mathrm{d}q \\ &= \mathrm{Tr}[\hat{\rho}].\end{aligned} \tag{4.22}$$

The claim follows from the fact that $\mathrm{Tr}[\hat{\rho}] = 1$. □

To prove the negativeness property of the Wigner function we start with the following key property of the Wigner function.

Proposition 4.1 (Trace)**.** *The trace of the product of two operators in Hilbert space is given by the multiplication of the inverse Weyl transformations integrated over the whole phase space ,*

$$\mathrm{Tr}[\hat{A}\hat{B}] = \frac{1}{2\pi\hbar}\iint A_w(q,p)B_w(q,p)\mathrm{d}q\mathrm{d}p. \tag{4.23}$$

Proof.

$$\begin{aligned}\iint A_w(q,p)B_w(q,p)\mathrm{d}q\mathrm{d}p &= \iiiint e^{-ip\frac{y+y'}{\hbar}} \langle q+\frac{y}{2}|\,\hat{A}\,|q-\frac{y}{2}\rangle \langle q+\frac{y'}{2}|\,\hat{B}\,|q-\frac{y'}{2}\rangle\,\mathrm{d}q\mathrm{d}p\mathrm{d}y\mathrm{d}y' \\ &= 2\pi\hbar\iiint \delta(y-y')\,\langle q+\frac{y}{2}|\,\hat{A}\,|q-\frac{y}{2}\rangle \langle q+\frac{y'}{2}|\,\hat{B}\,|q-\frac{y'}{2}\rangle\,\mathrm{d}q\mathrm{d}y\mathrm{d}y' \\ &= 2\pi\hbar\iint \langle q+\frac{y}{2}|\,\hat{A}\,|q-\frac{y}{2}\rangle \langle q-\frac{y}{2}|\,\hat{B}\,|q+\frac{y}{2}\rangle\,\mathrm{d}q\mathrm{d}y.\end{aligned} \tag{4.24}$$

In the first step we integrated over p giving the delta function which is used in evaluating the y' integral in the second step. As a last step we make the following change of variables

$$\begin{aligned} u &= q-\frac{y}{2}, \\ v &= q+\frac{y}{2}, \\ \mathrm{d}u\mathrm{d}v &= \mathrm{d}q\mathrm{d}y. \end{aligned} \tag{4.25}$$

Applying this change of variables we find that,

$$\begin{aligned}\iint A_w(q,p)B_w(q,p)\mathrm{d}q\mathrm{d}p &= 2\pi\hbar\iint \langle v|\,\hat{A}\,|u\rangle \langle u|\,\hat{B}\,|v\rangle\,\mathrm{d}u\mathrm{d}v \\ &= 2\pi\hbar\mathrm{Tr}[\hat{A}\hat{B}].\end{aligned} \tag{4.26}$$

□

This is an important proposition as it will turn out to be very useful for calculating expectation values of operators and help us prove many properties of the Wigner function.

We calculate expectation values by substituting $\hat{B}=\hat{\rho}$ in (4.23) and using proposition 2.10. It yields

$$\langle\hat{A}\rangle = \iint \rho_W(q,p)A_w(q,p)\mathrm{d}q\mathrm{d}p. \tag{4.27}$$

Claim. *The Wigner distribution function does not satisfy the nonnegative condition* (4.2).

For two pure states $|\psi_a\rangle$ and $|\psi_b\rangle$ let $\hat{\rho}_a$ and $\hat{\rho}_b$ be the corresponding density operators. The trace of the product of two density operators is given by,

$$\mathrm{Tr}[\hat{\rho}_a\hat{\rho}_b] = |\langle\psi_a|\psi_b\rangle|^2\,. \tag{4.28}$$

By proposition 4.1 we find that

$$2\pi\hbar\iint \rho_{W,a}(q,p)\rho_{W,b}(q,p)\mathrm{d}q\mathrm{d}p = |\langle\psi_a|\psi_b\rangle|^2\,. \tag{4.29}$$

When the pure states are orthogonal states we find

$$\iint \rho_{W,a}(q,p)\rho_{W,b}(q,p)\mathrm{d}q\mathrm{d}p = 0. \tag{4.30}$$

This means that some Wigner functions ρ_W must have both regions in phase space where it attains negative values as well as positive values. For this reason we can not interpret the Wigner function as a probability distribution. We rather speak of a so called quasiprobability distribution, which allows for negative values.

Claim. *The Wigner function is bounded and an upper bound is given by* $\frac{1}{\pi\hbar}$.

Proof. For a pure state $\hat{\rho} = |\Psi\rangle \langle\Psi|$

$$
\begin{aligned}
|\rho_W(q,p)| &= \left|\frac{1}{2\pi\hbar}\int e^{-i\frac{py}{\hbar}}\,\langle q+\frac{y}{2}|\,\hat{\rho}\,|q-\frac{y}{2}\rangle\,\mathrm{d}y\right| \\
&= \left|\frac{1}{\pi\hbar}\int e^{-i\frac{py}{\hbar}}\,\langle q+\frac{y}{2}|\,\hat{\rho}\,|q-\frac{y}{2}\rangle \mathrm{d}(\frac{1}{2}y)\right| \\
&= \left|\frac{1}{\pi\hbar}\int \Psi_1(y')^*\Psi_2(y')\mathrm{d}(y')\right| \\
&\le \frac{1}{\pi\hbar}.
\end{aligned} \tag{4.31}
$$

In the first step we changed the integration over $\frac{1}{2}y$ which results in an additional factor two. In the second step we introduced the normalized wave functions

$$
\begin{aligned}
\Psi_1(y') &= e^{+2i\frac{py'}{\hbar}}\Psi(q-y'), \\
\Psi_2(y') &= \Psi(q+y').
\end{aligned} \tag{4.32}
$$

In the last step we use the Cauchy-Schwarz inequality (2.7).

The claim stays to be to proved for mixed states. The Wigner distribution function has the key advantage that it has an easy generalisation to mixed states which we state in the following proposition.

Proposition 4.2 (Wigner distribution for mixed states)**.** *Let $\hat{\rho}$ describe a mixed state which is represented in terms of the pure states Ψ_j with coeficients P_j by*

$$
\hat{\rho} = \sum_j P_j\,|\Psi_j\rangle\,\langle\Psi_j|\,, \tag{4.33}
$$

then the Wigner distribution function of $\hat{\rho}$ is given by

$$
\rho_W(q,p) = \sum_j P_j\rho_{W,j}(q,p), \tag{4.34}
$$

where $\rho_{W,j}(q,p)$ is the Wigner distribution function corresponding to the pure state given by

$$
\hat{\rho}_j = |\Psi_j\rangle\,\langle\Psi_j|\,. \tag{4.35}
$$

Proof. The proof follows directly from the bilinearity of the Wigner distribution function. □

From (4.34) and the previous result for a pure states $\rho_{W,j}(q,p) \le \frac{1}{\pi\hbar}$ the boundedness for mixed states follow

$$
\begin{aligned}
\rho_W(q,p) &= \sum_j P_j\rho_{W,j}(q,p), \\
&\le \frac{1}{\pi\hbar}\sum_j P_j, \\
&= \frac{1}{\pi\hbar}.
\end{aligned} \tag{4.36}
$$

□

For a pure state which is either even or odd this bound is attained in the origin. The value of the Wigner function in the origin is given by

$$
\rho_W(0,0) = \frac{1}{2\pi\hbar}\int \langle\frac{y}{2}|\,\hat{\rho}\,|{-\frac{y}{2}}\rangle\,\mathrm{d}y. \tag{4.37}
$$

Even states satisfy $\langle \frac{y}{2}|\psi\rangle = \langle -\frac{y}{2}|\psi\rangle$, substituting this into equation (4.37) gives

$$\rho_W(0,0) = \frac{1}{\pi\hbar}\mathrm{Tr}[\hat{\rho}] = \frac{1}{\pi\hbar}. \tag{4.38}$$

This has as result that the Wigner function $\rho_W(q,p)$ has a peak with value $\frac{1}{\pi\hbar}$ at the origin. Similar for odd states this means that the Wigner function $\rho_W(q,p)$ has a minimum at the origin with value of $-\frac{1}{\pi\hbar}$. This confirms our previous claim that the Wigner distribution function can attain negative values.

Claim. *The Wigner function is Galilei invariant in position and in momentum coordinate*

With Galilei invariant we mean the property when the state $\Psi(q) \to \Psi(q-a)$ due to an Galilean transformation results in a similar shift in the Wigner density function $\rho_W(q,p) \to \rho_W(q-a,p)$. A similar result holds for the momentum coordinate.

Proof. For a pure state $\hat{\rho} = |\Psi\rangle\langle\Psi|$ the Wigner function in (4.16) can be written as,

$$\rho_W(q,p) = \frac{1}{2\pi\hbar}\int e^{-i\frac{py}{\hbar}}\Psi(q+\frac{y}{2})\Psi^*(q-\frac{y}{2})\mathrm{d}y. \tag{4.39}$$

It now follows directly from (4.39) that a change in position $\Psi(q) \to \Psi(q-a)$ gives the same shift in the Wigner function $\rho_W(q,p) \to \rho_W(q-a,p)$.

Similar for momentum, to shift the momentum of Ψ by $+b_p$ we get that $\Psi(q) \to \Psi(q)e^{ib_p\frac{q}{\hbar}}$. A direct substitution in (4.39) gives that $\rho_W(q,p) \to \rho_W(q,p-b_p)$. In the case of mixed states, $\Psi_j(q) \to \Psi_j(q-a)$ for all j has the result $\rho_W(q,p) \to \rho_W(q-a,p)$. This follows directly from (4.34). From this we conclude that the Wigner function is Galilei invariant. □

O'Connel and Wigner [18] proved that the Wigner distribution function is unique if one require the distribution function to be a real valued bilinear distribution function which is Galilei invariant and satisfy the correct marginals.

4.3 Minimum uncertainty states

A minimum uncertainty state is a state which satisfies the equality of the uncertainty relation (2.4) for position and momentum. In this section we will take a look at these states and their corresponding Wigner functions.

Claim. *Every minimum uncertainty state corresponds to a nonnegative Wigner function.*

4.3.1 General uncertainty principle

To prove this claim we start by first investigating what type of states have minimum uncertainty. We start by deriving the general uncertainty principle and look what inequalities we use. To prove the general uncertainty principle we follow the approach taken by Griffiths [7]. For any observables $\hat{A}$ and $\hat{B}$ define,

$$|f\rangle = |(\hat{A} - \langle\hat{A}\rangle)\Psi\rangle\,, \tag{4.40a}$$

$$|g\rangle = |(\hat{B} - \langle\hat{B}\rangle)\Psi\rangle\,, \tag{4.40b}$$

such that the variance is given by

$$\sigma_A^2 = \langle f|f\rangle\,, \tag{4.41a}$$

$$\sigma_B^2 = \langle g|g\rangle\,. \tag{4.41b}$$

The first inequality we use is the Cauchy-Schwarz inequality (2.7) which gives us

$$\sigma_A^2\sigma_B^2 = \langle f|f\rangle\langle g|g\rangle \geq |\langle f|g\rangle|^2\,. \tag{4.42}$$

The second inequality is obtained by dropping the real part of $\langle f|g\rangle$ which results in,

$$\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}(\langle f|g\rangle - \langle g|f\rangle)\right)^2. \tag{4.43}$$

Straight forward algebra of substituting equations (4.40) into (4.43) results in the generalized uncertainty principle given by,

$$\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2. \tag{4.44}$$

Definition 4.3 (Minimum uncertainty state)**.** *The state Ψ is called a minimum uncertainty state if the uncertainty in Ψ given by* (4.44) *with respect to the position and momentum operator, respectively $\hat{q}$ and $\hat{p}$, becomes an equality.*

To find the general expression for minimum uncertainty states we need to find the situations in which the two above used inequalities become equalities, and solve for Ψ. The Cauchy-Schwarz inequality becomes a non trivial equality if one of the functions is a multiple of the other, in our case when $g(x) = cf(x)$ with $c \in \mathbb{C}$. In the second inequality we dropped the real part of $\langle f|g\rangle$. The only way for this to become an equality is when the real part is exactly zero. This means that

$$\mathrm{Re}(\langle f|g\rangle) = \mathrm{Re}(c\,\langle f|f\rangle) = 0. \tag{4.45}$$

As $\langle f|f\rangle$ is real the only way to satisfy this equality is when $\mathrm{Re}(c) = 0$. We conclude that a state has minimum uncertainty if and only if it satisfies (4.46),

$$g(x) = iaf(x), a \in \mathbb{R}. \tag{4.46}$$

For the momentum and position operator this gives us the following differential equation

$$\left(\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x} - \langle\hat{p}\rangle\right)\Psi = ia(x - \langle\hat{x}\rangle)\Psi. \tag{4.47}$$

Equation (4.47) is a first order differential equation. Its general solution is given by

$$\Psi(x) = Ae^{-a\frac{(x-\langle\hat{x}\rangle)^2}{2\hbar} + i\langle\hat{p}\rangle\frac{x}{\hbar}}. \tag{4.48}$$

This is an important result. Minimum uncertain states have as general form a Gaussian function displaced such that the expectation values for position is given by $\langle\hat{x}\rangle$ and momentum $\langle\hat{p}\rangle$. The result that every minimum uncertainty state is of Gaussian form has as a consequence that mixed states can never obtain the minimum uncertainty limit. This is a direct consequence of the fact that two different Gaussian functions are never orthogonal to each other [8].

4.3.2 Wigner distribution function of a Gaussian

As proven in previous section the Wigner function is not necessary everywhere positive. For pure states we can classify which type wave functions give rise to a positive Wigner function. Hudson proved that the Wigner function for a pure state is nonnegative if and only if the wave function is a Gaussian function [19].

Proposition 4.3. *The Wigner distribution function corresponding to the pure state Ψ in Hilbert space is nonnegative if and only if Ψ is a Gaussian, that is if it can be written in the form of* (4.49)*,*

$$\Psi(q) = e^{-\frac{1}{2}(aq^2+2bq+c)}, \mathrm{Re}(a) > 0, \tag{4.49}$$

where a, b, c are constants in $\mathbb{C}$ such that the wave function is a correctly normalized wave function in Hilbert space.

Proof. We will prove the sufficiency by direct computation. In section 5 where we introduce the Husimi distribution the following results will come in handy. We will show the statement for a slightly less general and for our purposes more convenient form of the wave function. Assume Ψ has the form given by

$$\Psi(q) = (2\pi a^2)^{-\frac{1}{4}} e^{\frac{(q-q_0)^2}{4a^2} + i\frac{p_0 q}{\hbar}}, \tag{4.50}$$

which is the general normalized Gaussian wave function displaced by (q_0, p_0). Substituting this equation in (4.39) gives the Wigner function given by [8],

$$\rho_W(q,p) = \frac{1}{\pi\hbar} e^{-\frac{(q-q_0)^2}{2(\Delta q)^2} - \frac{(p-p_0)^2}{2(\Delta p)^2}}. \tag{4.51}$$

Here we made use of short notation $\Delta q = a$ and $\Delta p = \frac{\hbar}{2a}$. Equation (4.51) is a multivariate normal distribution, from which we conclude that $\rho_W(q,p)$ for a Gaussian wave function is nonnegative for all (q,p).

For the converse direction we follow the approach of Hudson [19]. Let Ψ be a normalised wave function in Hilbert space and assume ρ_W to be the nonnegative probability distribution. Let $\rho_{W,z}$ denote the Wigner distribution function corresponding to the wave function given by

$$\Psi_z(q) = Ae^{-\frac{1}{2}q^2 + zq}, z \in \mathbb{C}. \tag{4.52}$$

With A the normalisation constant given by (4.53) and z an parameter in $\mathbb{C}$

$$|A(z)|^2 = \sqrt{\frac{1}{\pi}} e^{-Re(z)^2}. \tag{4.53}$$

Define the following function,

$$F(z) = \int \Psi^* e^{-\frac{1}{2}q^2 + zq} \mathrm{d}q = \frac{1}{A(z)} \langle \Psi | \Psi_z \rangle. \tag{4.54}$$

Clearly $F(z)$ is an entire function, we now intend to write $F(z)$ in its canonical form given by,

$$F(z) = e^{g(z)} z^m \Pi_j (1 - \frac{z}{z_j}) e^{P_j\left(\frac{z}{z_j}\right)}. \tag{4.55}$$

In this equation the non zero zeros of $F(z)$ are given by z_j and m the multiplicity of the zero at the origin, $g(z)$ is the polynomial with order of the genus and the function $P_j(z)$ is given by [20]

$$p_j(z) = \sum_{k=1}^{j} \frac{z^k}{k}, \tag{4.56}$$

From (4.29) we know that,

$$2\pi\hbar \iint \rho_W(q,p)\rho_{W,z}(q,p)\mathrm{d}q\mathrm{d}p = |\langle \Psi | \Psi_z \rangle|^2. \tag{4.57}$$

By assumption $\rho_W(q,p)$ is nonnegative for all (q,p). We just proved that the Wigner function of Gaussian wave functions, $\rho_{W,z}(q,p)$, are also positive for all z. From this we conclude that the left hand side of (4.57) is greater than zero, and thus $F(z)$ has no zeroes.

Using the Cauchy-Schwarz inequality (2.7) and (4.53) we find that,

$$|F(z)|^2 \leq \langle \Psi | \Psi \rangle \sqrt{\pi} e^{Re(z)^2}. \tag{4.58}$$

The order of $F(z)$ is given by the smallest value of λ such that $\forall \epsilon > 0$ we have that

$$|F(z)| \leq e^{|z|^{\lambda+\epsilon}}. \tag{4.59}$$

From equation (4.58) we conclude that the order is not bigger than two, and thus the order of the polynomial $g(z)$ in (4.55) is equal to two. If we combine the above results we can write $F(z)$ now in canonical form given by,

$$F(z) = e^{\alpha z^2 + \beta z + \gamma}. \tag{4.60}$$

If we now look at the special case $z = iy$ substituting in (4.54) and (4.60) we find,

$$e^{-\alpha y^2 + i\beta y + \gamma} = \int \left(\Psi^\dagger e^{-\frac{1}{2}q^2} \right) e^{-iyq} \mathrm{d}q. \tag{4.61}$$

We note that the right hand side is the Fourier transform of the function

$$h(q) = \Psi(q)^\dagger e^{-\frac{1}{2}q^2}. \tag{4.62}$$

Because the only functions which Fourier transform are Gaussian functions are Gaussian functions itself, it follows that $\Psi(q)$ must be a Gaussian function. Which concludes the proof of the proposition. □

Combining the results of section 4.3.1 and proposition 4.3 proves the claim stated at the beginning of the section. Every minimum uncertainty state has a nonnegative Wigner distribution function.

We have now introduced the Wigner function with all of its common properties. Further applications and the time dependence of the Wigner function will be discussed in section 7 and 6.

5 Husimi distribution

We finally arrive to the point were we look at the Husimi distribution. The Husimi distribution has the property that it is a positive definite distribution function. For the introduction of the Husimi distribution we follow the approach of [8].

Before we introduce the Husimi distribution lets us go through how we defined the probability distribution in configuration space. We started with a basis of position eigenvectors, denoted by $\{|q\rangle\}$. These eigenvectors form a complete orthonormal basis. The probability distribution P in position space for a state $\hat{\rho}$ is now given by

$$P(q) = \langle q|\hat{\rho}|q\rangle \,. \tag{5.1}$$

A similar construction exist for the probability distribution in momentum space. However now, we are looking for a probability distribution for both position and momentum. The problem which arises once we work in phase space is that there do not exist eigenvectors which are simultaneous position and momentum eigenvectors as $\hat{q}$ and $\hat{p}$ do not commute. The idea behind the Husimi distribution is to use the next closest basis, the minimum uncertainty states. We already encountered minimum uncertainty states in (4.48). We will denote these minimum uncertainty states located at the point (q, p) by the vector $|q, p\rangle$. Calculating the constant A and renaming variables of equation (4.48) in a more convenient way we find

$$\langle x|q,p\rangle = (2\pi s^2)^{-\frac{1}{4}} e^{-\frac{(x-q)^2}{4s^2} + i\frac{px}{\hbar}} \,. \tag{5.2}$$

Equation (5.2) is the general form of a Gaussian located at the point (q, p) with root mean square half-widths given by

$$\Delta q = s, \tag{5.3a}$$

$$\Delta p = \frac{\hbar}{2s}. \tag{5.3b}$$

It can be easily seen that this state has indeed minimum uncertainty, $\Delta q \Delta p = \frac{1}{2}\hbar$. These states described by (5.2) represent a squeezed state. Using these states as basis we find that they are normalized and form an overcomplete set, the proof is given by Ballentine [8]. We have the following overcompleteness relation

$$\iint |q,p\rangle \langle q,p| \, \mathrm{d}q\mathrm{d}p = 2\pi\hbar. \tag{5.4}$$

For every choice of s the set $\{|q,p\rangle\}$ spans a different basis. If we make a specif choice for s given by

$$s = \sqrt{\frac{\hbar}{2m\omega}}, \tag{5.5}$$

we find the coherent states $|\alpha\rangle$.

Recall that the coherent states for an overcomplete basis (2.40) which agrees with (5.4)

$$\frac{1}{\pi}\int \mathrm{d}^2\alpha \, |\alpha\rangle \langle\alpha| = \frac{1}{2\pi\hbar}\int \mathrm{d}q\mathrm{d}p \, |\alpha\rangle \langle\alpha| = \hat{\mathbb{1}}, \tag{5.6}$$

From now and onwards we fix s.

Definition 5.1 (Husimi distribution)**.** *The Husimi distribution is defined for the state $\hat{\rho}$ as*

$$\rho_H(q,p) = \frac{1}{(2\pi\hbar)} \langle q,p|\hat{\rho}|q,p\rangle \,. \tag{5.7}$$

This definition is very similar as how we defined the probability distribution in position or momentum space. A key difference is the factor $(2\pi\hbar)$, which is due the overcompleteness of the used basis. The Husimi distribution $\rho_H(q,p)$ can be interpreted as the probability that the state is in the region in phase space centered at (q,p) with uncertainty given by (5.3). In the limit $s \to 0$ the uncertainty in position becomes infinitely small. This has as result that the minimum uncertainty states given by (5.2) approximate a position eigenstates. The Husimi distribution reduces to the probability distribution given in position space. Similar in the limit $s \to \infty$ the uncertainty states approximate momentum eigenstates and the Husimi distribution represents the probability distribution in momentum space. The parameter s of the Husimi distribution determines the relative resolution in position and momentum space. The Q-distribution can be obtained by making a specific choice for the parameter s.

We begin by noting that also the Husimi distribution is bilinear in the wave function.

Claim. *The Husimi distribution is bilinear in the wave function*

This follows just as for the Wigner distribution function directly from the bilinear form of $\hat{\rho}$. As a consequence the Husimi distribution, just as the Wigner distribution function, can not both satisfy the marginal condition (4.1) and the nonnegative condition (4.2). For this reason we also refer to the Husimi distribution as a quasi probability distribution.

Claim. *The Husimi distribution is normalized over phase space.*

Proof. We will show the statement for a pure state given by $\hat{\rho} = |\Psi\rangle\langle\Psi|$. The generalisation for mixed states is straightforward. We first look at the position marginal $P_H(q)$ of the Husimi distribution

$$\begin{aligned} P_H(q) &= \int \rho_H(q,p)\mathrm{d}p \\ &= \frac{1}{2\pi\hbar}\int \langle q,p|\hat{\rho}|q,p\rangle\, \mathrm{d}p \\ &= \frac{1}{2\pi\hbar}\iiint \langle q,p|x\rangle\langle x|\Psi\rangle\langle\Psi|x'\rangle\langle x'|q,p\rangle\, \mathrm{d}p\mathrm{d}x\mathrm{d}x' \\ &= \frac{1}{2\pi\hbar}\iiint \langle x|\Psi\rangle\langle\Psi|x'\rangle\,(2\pi s^2)^{-\frac{1}{2}}e^{\frac{1}{4s^2}((q-x)^2+(q-x')^2)}e^{i\frac{p}{\hbar}(x-x')}\mathrm{d}p\mathrm{d}x\mathrm{d}x'. \end{aligned} \tag{5.8}$$

Here we substituted in the first step two identity operators $\hat{\mathbb{1}} = \int |x\rangle\langle x|\,\mathrm{d}x$ and used equation (5.2) in the last step. For the next step we integrate over the p variable, this will give us an $2\pi\hbar\delta(x-x')$ term. Finally integrating over x' gives us the result

$$P_H(q) = \int (2\pi s^2)^{-\frac{1}{2}}e^{\frac{1}{4s^2}(q-x)^2}\,|\langle x|\Psi\rangle|^2\mathrm{d}x \tag{5.9}$$

We now are in the position to actually calculate our wanted expression for the normalisation

$$\begin{aligned} \iint \rho_H(q,p)\mathrm{d}q\mathrm{d}p &= \int P_H(q)\mathrm{d}q, \\ &= \iint (2\pi s^2)^{-\frac{1}{2}}e^{\frac{1}{4s^2}(q-x)^2}\,|\langle x|\Psi\rangle|^2\mathrm{d}x\mathrm{d}q, \\ &= \int |\langle x|\Psi\rangle|^2\mathrm{d}x. \end{aligned} \tag{5.10}$$

In the first step we did the integration over the q variable. Due to the normalisation of $\langle q,p|q,p\rangle$ the terms coming from the uncertainty wave packet gives the identity. And thus we find the desired result by simply doing the integration over x and noting that Ψ is integrated normalized.

$$\iint \rho_H(q,p)\mathrm{d}q\mathrm{d}p = 1. \tag{5.11}$$

□

Claim. *The Husimi distribution satisfies the nonnegative condition* (4.2).

Proof. We again show this only for a pure state as the generalisation to mixed states is straightforward. For the state $\hat{\rho} = |\Psi\rangle\langle\Psi|$, by definition we have the Husimi distribution given by

$$\begin{aligned}\rho_H(q,p) &= \frac{1}{2\pi\hbar}\langle q,p|\hat{\rho}|q,p\rangle \\ &= \frac{1}{2\pi\hbar}|\langle q,p|\Psi\rangle|^2 \\ &\geq 0.\end{aligned} \tag{5.12}$$

□

Just as the Wigner distribution the Husimi distribution is bounded.

Claim. *The Husimi distribution is bounded between* $0 \leq \rho_H \leq \frac{1}{2\pi\hbar}$.

Proof. The lower bound follows from the previous claim. The upper bound follows from the fact that $\langle q,p|\hat{\rho}|q,p\rangle \leq 1$. □

Claim. *The Husimi distribution does not satisfy the marginal condition* (4.1)

Proof. We show this by looking at a pure state $\hat{\rho} = |\Psi\rangle\langle\Psi|$ and calculating the marginal for position and show it does not satisfy the correct value. We already calculated above the marginal distribution for position given by (5.9)

$$P_H(q) = \int (2\pi s^2)^{-\frac{1}{2}} e^{\frac{1}{4s^2}(q-x)^2} |\langle x|\Psi\rangle|^2 \mathrm{d}x. \tag{5.13}$$

It follows that $P_H(q) \neq |\langle q|\Psi\rangle|^2$ as desired. □

In fact the Husimi marginal probability distribution is the Gaussian broadened version of the wanted marginal distribution $|\langle q|\Psi\rangle|^2$. In the case when $s \to 0$ the Gaussian function becomes an delta function at q. In this limit we find for the marginal

$$\lim_{s\to 0} P_H(q) = |\langle q|\Psi\rangle|^2. \tag{5.14}$$

As we deduced in the begin of this paragraph. A similar derivation holds for the marginal distribution in momentum representation.

Claim. *The Husimi distribution is a Gaussian smoothing of the Wigner distribution function [21].*

Proof. We start by rewriting $\langle q,p|\hat{\rho}|q,p\rangle = \mathrm{Tr}[|q,p\rangle\langle q,p|\,\hat{\rho}]$. If we now use the inverse Weyl transform to calculate the trace using proposition 4.1 we find

$$\rho_H(q,p) = \frac{1}{2\pi\hbar}\mathrm{Tr}[|q,p\rangle\langle q,p|\,\hat{\rho}] \tag{5.15}$$

$$= \left(\frac{1}{2\pi\hbar}\right)^2 \iint (|q,p\rangle\langle q,p|)_w(q',p')\rho_w(q',p')\mathrm{d}q'\mathrm{d}p', \tag{5.16}$$

were the subscript w denotes the inverse Weyl transform. Now using the relation of the inverse Weyl transform to the Wigner function we find

$$\rho_H(q,p) = \iint \rho_{W,qp}(q',p')\rho_W(q',p')\mathrm{d}q'\mathrm{d}p'. \tag{5.17}$$

Here ρ_W denotes the Wigner distribution function and $\rho_{W,qp}$ denotes the Wigner distribution function of the state given by $\hat{\rho}_{qp} = |q,p\rangle\langle q,p|$. We actually already calculated $\rho_{W,qp}$ before, this is namely precisely what we calculated in (4.51)

$$\rho_{W,qp}(q',p') = \frac{1}{\pi\hbar} e^{-\frac{(q'-q)^2}{2s^2} - \frac{2s^2(p'-p)^2}{\hbar^2}}, \tag{5.18}$$

where $\Delta q = s$ and $\Delta p = \frac{\hbar}{2s}$. Notice that $\rho_{W,qp}(q,p)$ is a Gaussian in both position and momentum. Thus equation (5.17) can be interpreted as a Gaussian smoothing of the Wigner distribution function. □

This means that once we have the Wigner distribution function we can simply calculate the Husimi distribution by smoothing with a minimum uncertainty Gaussian. One can find the Q-distribution as a special case of the Husimi distribution [6]. For the specific choice of s given by (5.5) the state described by (5.2) reduces to the coherent states. The uncertainty in Δq and Δp are given by (2.41)

$$\Delta q = \sqrt{\frac{\hbar}{2m\omega}}, \tag{5.19a}$$

$$\Delta p = \sqrt{\frac{\hbar m\omega}{2}}, \tag{5.19b}$$

we find that the Husimi distribution gives the Q-distribution for this choice.

Just as for the Wigner distribution function, we are interested in calculating expectation values. We calculated expectation values with the Wigner function making use of the Weyl transform. In a similar way there exist a different transform which is used to calculate expectation values with the Husimi distribution function. We will not go into detail but for completeness we will give the general formula derived by Lee [6]. The expectation value of an operator $\hat{A}(\hat{q},\hat{p})$ is given by

$$\mathrm{Tr}[\hat{\rho}\hat{A}] = \iint A_h(q,p)\rho_H(q,p)\mathrm{d}q\mathrm{d}p. \tag{5.20}$$

Where $A_h(q,p)$ is the anti-Husimi transform of the operator $\hat{A}(\hat{q},\hat{p})$ given by

$$A_h(q,p) = \frac{1}{4\pi^2} \iint \mathrm{Tr}[\hat{A}(\hat{q},\hat{p}) e^{i\xi\hat{q}+i\eta\hat{p}} e^{\frac{s^2\xi^2}{2}+\hbar^2\frac{\eta^2}{8s^2}}]\mathrm{d}\xi\mathrm{d}\eta. \tag{5.21}$$

6 Particle in a box

In this section we will take a look at an explicit example of a particle in a box. We will take a look at the Wigner distribution function and the Husimi distribution corresponding to this problem. Let us first define the problem.

We look at a free particle of mass m bounded by the following potential

$$V(q) = \begin{cases} 0 & \text{if } 0 \leq q \leq a, \\ \infty & \text{elsewhere.} \end{cases} \tag{6.1}$$

This potential corresponds to an infinite potential well with ends at $q = 0$ and $q = a$. This example is well discussed in many introduction courses for quantum mechanics, for example in [7] and [22]. The energy eigenvalues of the n^{th} excited state are given by

$$E_n = \tfrac{n^2\pi^2\hbar^2}{2ma^2}, \qquad\qquad n = 1, 2, 3, \ldots \tag{6.2}$$

The position eigenstates are given by

$$\langle q|\Psi_n\rangle = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}q\right) & \text{if } 0 \leq q \leq a, \\ 0 & \text{elsewhere.} \end{cases} \tag{6.3}$$

The corresponding momentum space eigenstates are given by

$$\langle p|\Psi_n\rangle = (-i)\sqrt{\frac{a}{\pi\hbar}} e^{-ip\frac{a}{2\hbar}} \left(e^{+i\frac{n\pi}{2}} \frac{\sin\left(p\frac{a}{2\hbar} - \frac{n\pi}{2}\right)}{p\frac{a}{\hbar} - n\pi} - e^{-i\frac{n\pi}{2}} \frac{\sin\left(p\frac{a}{2\hbar} + \frac{n\pi}{2}\right)}{p\frac{a}{\hbar} + n\pi} \right). \tag{6.4}$$

For later illustrative purposes we also give the probability densities

$$|\langle q|\Psi_n\rangle|^2 = \begin{cases} \frac{2}{a} \sin^2\left(\frac{n\pi}{a}q\right) & \text{if } 0 \leq q \leq a, \\ 0 & \text{elsewhere.} \end{cases} \tag{6.5}$$

$$|\langle p|\Psi_n\rangle|^2 = \frac{a}{\pi\hbar} \left(\frac{\sin^2\left(p\frac{a}{2\hbar} - \frac{n\pi}{2}\right)}{\left(p\frac{a}{\hbar} - n\pi\right)^2} + \frac{\sin^2\left(p\frac{a}{2\hbar} + \frac{n\pi}{2}\right)}{\left(p\frac{a}{\hbar} + n\pi\right)^2} - 2\cos(n\pi) \frac{\sin\left(p\frac{a}{2\hbar} - \frac{n\pi}{2}\right)\sin\left(p\frac{a}{2\hbar} + \frac{n\pi}{2}\right)}{(p\frac{a}{\hbar} + n\pi)(p\frac{a}{\hbar} - n\pi)} \right) \tag{6.6}$$

6.1 Wigner distribution of the infinite potential well

The Wigner distribution function for the n^{th} energy eigenstate can be calculated by (4.16). We used the substitution $y = \frac{1}{2}y'$ and made use of the fact that the position eigenstates are real.

$$\rho_W^n(q,p) = \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} \langle q+y|\Psi_n\rangle \langle q-y|\Psi\rangle\, e^{-2i\frac{py}{\hbar}}\, \mathrm{d}y. \tag{6.7}$$

To solve this integral we make use of the fact that $\langle q \pm y|\Psi_n\rangle$ vanishes outside the region of $[0, a]$. This means that the integral only does not vanish for the following conditions

$$0 \leq q + y \leq a, \tag{6.8a}$$
$$0 \leq q - y \leq a. \tag{6.8b}$$

In figure 1 these four conditions are illustrated. The integral is only non vanishing in the region enclosed by the red and blue lines. For $q \in [0, \frac{1}{2}a]$ the integration limits are the red lines. For $q \in [\frac{1}{2}a, a]$ the integration limits are the blue lines. With the help of the figure we conclude that the limits of the integral are given by

$$\begin{array}{ll} [-q, q] & \text{if } q \in [0, \frac{1}{2}a], \\ [-a+q, a-q] & \text{if } q \in [\frac{1}{2}a, a]. \end{array} \tag{6.9}$$

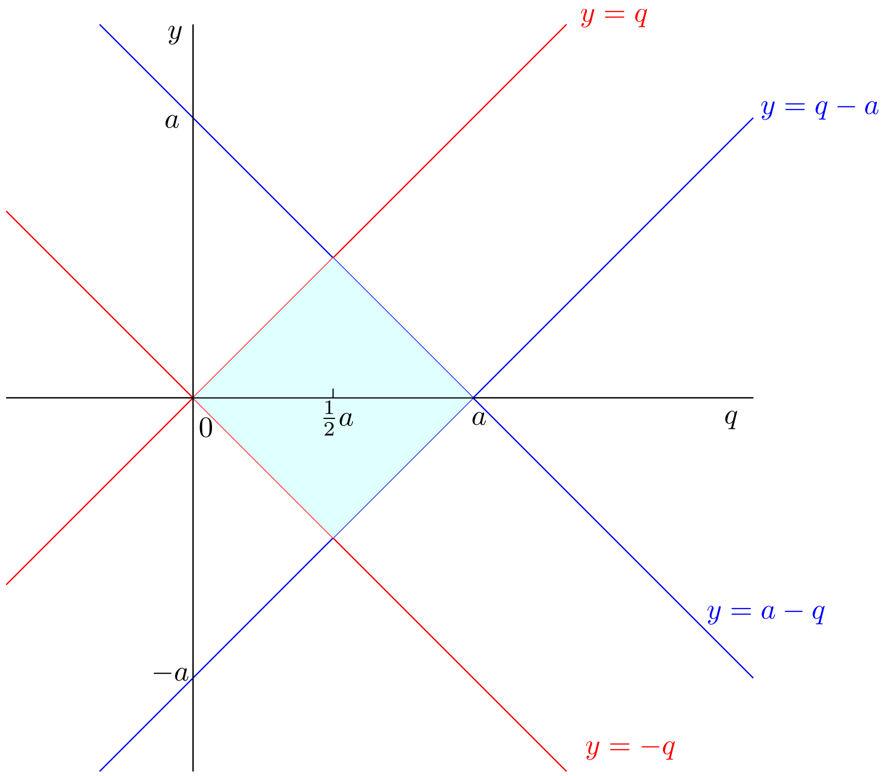

Figure 1: The conditions (6.8) displayed in the (q, y)-plane.

This helps us simplify the integral (6.7). We separate two different cases. In the case that $q \in [0, \frac{1}{2}a]$ we find for the Wigner distribution function

$$\rho_W^n(q,p) = \frac{1}{\pi\hbar}\int_{-q}^{q} \frac{2}{a}\sin\left(\frac{n\pi}{a}(q+y)\right)\cdot\sin\left(\frac{n\pi}{a}(q-y)\right)e^{-2i\frac{py}{\hbar}}\,\mathrm{d}y. \tag{6.10}$$

This integral is solved in the appendix B, the Wigner function for the n$^{\text{th}}$ energy eigenstate with $q \in [0, \frac{1}{2}a]$ is given by

$$\rho_W^n(q,p) = \left(\frac{2}{\pi\hbar a}\right)\left(\frac{\sin\left(2q(\frac{p}{\hbar}-\frac{n\pi}{a})\right)}{4(\frac{p}{\hbar}-\frac{n\pi}{a})} + \frac{\sin\left(2q(\frac{p}{\hbar}+\frac{n\pi}{a})\right)}{4(\frac{p}{\hbar}+\frac{n\pi}{a})} - \cos\left(\frac{2n\pi q}{a}\right)\frac{\sin\left(\frac{2pq}{\hbar}\right)}{\frac{2p}{\hbar}}\right). \tag{6.11}$$

For the other case when $q \in [\frac{1}{2}a, a]$ we make use of the symmetry in this specific problem. We need to solve the following integral

$$\rho_W^n(q,p) = \frac{1}{\pi\hbar}\int_{q-a}^{a-q} \frac{2}{a}\sin\left(\frac{n\pi}{a}(q+y)\right)\cdot\sin\left(\frac{n\pi}{a}(q-y)\right)e^{-2i\frac{py}{\hbar}}\,\mathrm{d}y. \tag{6.12}$$

If we now introduce the variable x as

$$x = a - q. \tag{6.13}$$

Using this substitution in equation (6.12) we find for $x \in [0, \frac{1}{2}a]$

$$\begin{aligned}
\rho_W^n(a-x,p) &= \frac{1}{\pi\hbar}\int_{-x}^{x} \frac{2}{a}\sin\left(\frac{n\pi}{a}(a-x+y)\right)\cdot\sin\left(\frac{n\pi}{a}(a-x-y)\right)e^{-2i\frac{py}{\hbar}}\,\mathrm{d}y \\
&= \frac{1}{\pi\hbar}\int_{-x}^{x} \frac{2}{a}(-1)^{2n+2}\sin\left(\frac{n\pi}{a}(x-y)\right)\cdot\sin\left(\frac{n\pi}{a}(x+y)\right)e^{-2i\frac{py}{\hbar}}\,\mathrm{d}y \\
&= \rho_W^n(x,p).
\end{aligned} \tag{6.14}$$

In the second step we made use of the properties that the sine is an odd function and for every phase shift of $n\pi$ the function gains a factor $(-1)^n$.

Concluding, the Wigner distribution function for the n^{th} eigenstate of a particle in a box is given by equation (6.11) if $q \in [0, \frac{1}{2}a]$ and is given by $\rho_W^n(q,p) = \rho_W^n(a-q,p)$ if $q \in [\frac{1}{2}a, a]$. This means that for all energy eigenstates the Wigner distribution is symmetric around the middle of the so called box. This symmetry in the Wigner distribution function is a direct consequence of the same symmetry in the infinite potential well.

6.1.1 Properties of the Wigner distribution function

To display the Wigner distribution function we first make our variables dimensionless by the following substitution

$$q' = \frac{q}{a}, \tag{6.15a}$$

$$p' = \frac{ap}{\hbar}, \tag{6.15b}$$

$$\rho'_W(q,p) = \hbar\rho_W(q,p). \tag{6.15c}$$

We start by looking at the Wigner distribution function for the ground state where $n = 1$ shown in figure 2.

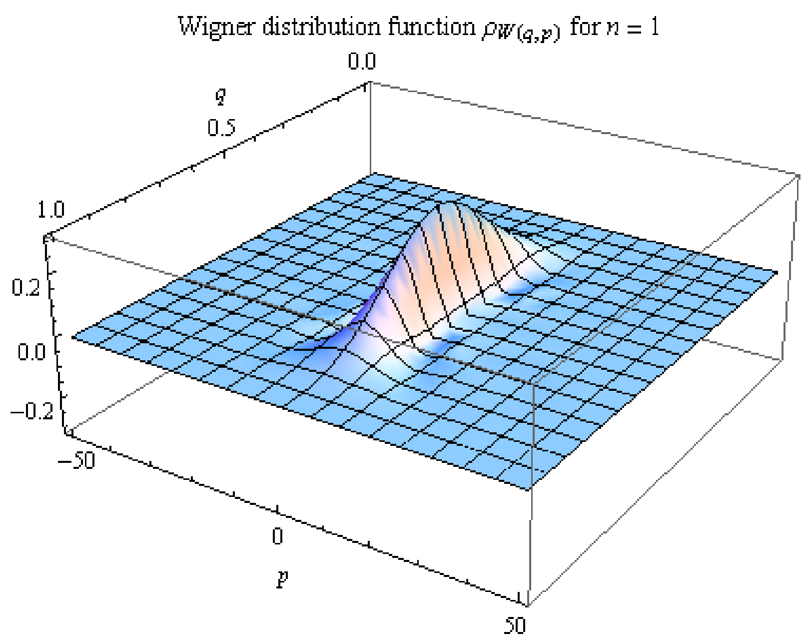

Figure 2: Wigner distribution function of the ground state of the infinite potential well in the scaled variables given by (6.15)

This example shows properties we discussed in section 4.2. First of all the Wigner distribution function is a real valued bounded but not strictly positive distribution. Although it is hard to see in figure 2 the Wigner distribution attains negative values. In figure 3 we have plot the negative parts of the Wigner distribution function.

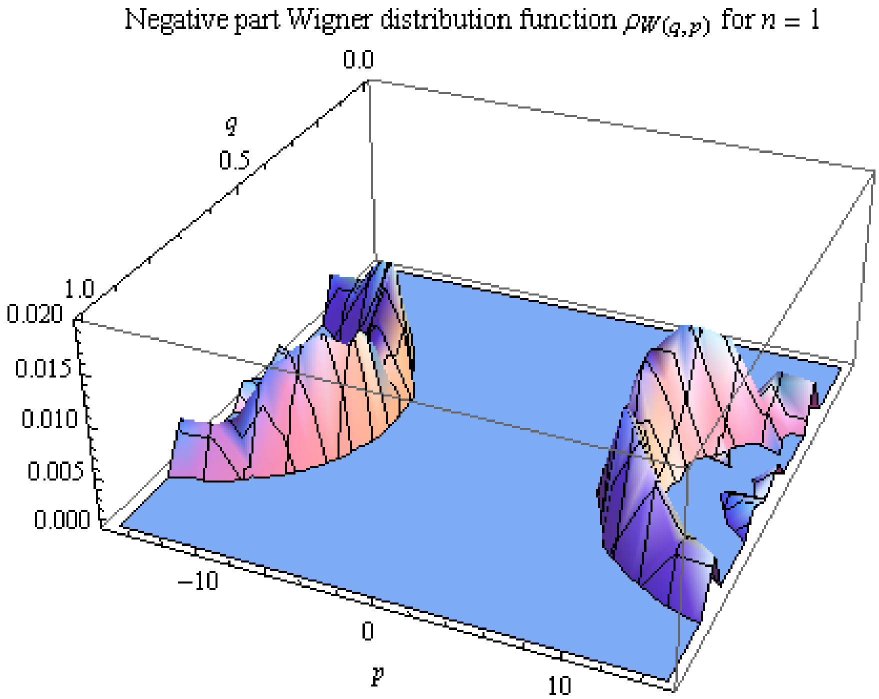

Figure 3: Negative part of the Wigner distribution function of the ground state of the infinite potential well in the scaled variables given by (6.15)

The wave function (6.3) is an even function around our scaled variable $q' = \frac{1}{2}$. As a result we find that the Wigner distribution function attains its maximum for $\rho_W(\frac{1}{2}, 0) = \frac{1}{\pi}$ similar to (4.38).

An other discussed property of the Wigner distribution function is that it is normalized *i.e.*

$$\iint \rho_W^n(q,p)\mathrm{d}q\mathrm{d}p = 1. \tag{6.16}$$

We can check this property by direct calculation. We first calculating the marginal distribution in position starting from equation (6.10)

$$\begin{aligned}
\int \rho_W^n(q,p)\mathrm{d}p =& \frac{1}{\pi\hbar}\int_{\infty}^{\infty}\int_{-q}^{q}\frac{2}{a}\sin\left(\frac{n\pi}{a}(q+y)\right)\cdot\sin\left(\frac{n\pi}{a}(q-y)\right)e^{-2i\frac{py}{\hbar}}\mathrm{d}y\mathrm{d}p && (6.17)\\
=&\int_{-q}^{q}\delta(y)\frac{2}{a}\sin\left(\frac{n\pi}{a}(q+y)\right)\cdot\sin\left(\frac{n\pi}{a}(q-y)\right)\mathrm{d}y && (6.18)\\
=&\frac{2}{a}\sin\left(\frac{n\pi}{a}q\right)^2. && (6.19)
\end{aligned}$$

In the first step the integration over p is carried out which gives the term $\pi\hbar\delta(y)$. We find the equation for the marginal distribution

$$\int \rho_W^n(q,p)\mathrm{d}p = |\langle q|\hat{\rho}\rangle|^2 = \frac{2}{a}\sin\left(\frac{n\pi}{a}(q)\right)^2. \tag{6.20}$$

Integration over q now proves the normalization.

6.1.2 Mixed states

One of the advantages of the phase space formalism is it generalizes to mixed states very easy.

Example 6.1 (Mixed state)**.** Lets for example look at the mixed state given by

$$\hat{\rho} = \frac{1}{2} \left(|\Psi_1\rangle \langle\Psi_1| + |\Psi_7\rangle \langle\Psi_7| \right), \tag{6.21}$$

where Ψ_1 and Ψ_7 are pure eigenstates of the discussed infinite potential well given by (6.3). Recall proposition 4.2 the Wigner distribution function of this mixed state is given by

$$\rho_W(q,p) = \frac{1}{2} \left(\rho_W^1(q,p) + \rho_W^7(q,p) \right). \tag{6.22}$$

This is illustrated in the following figure 4

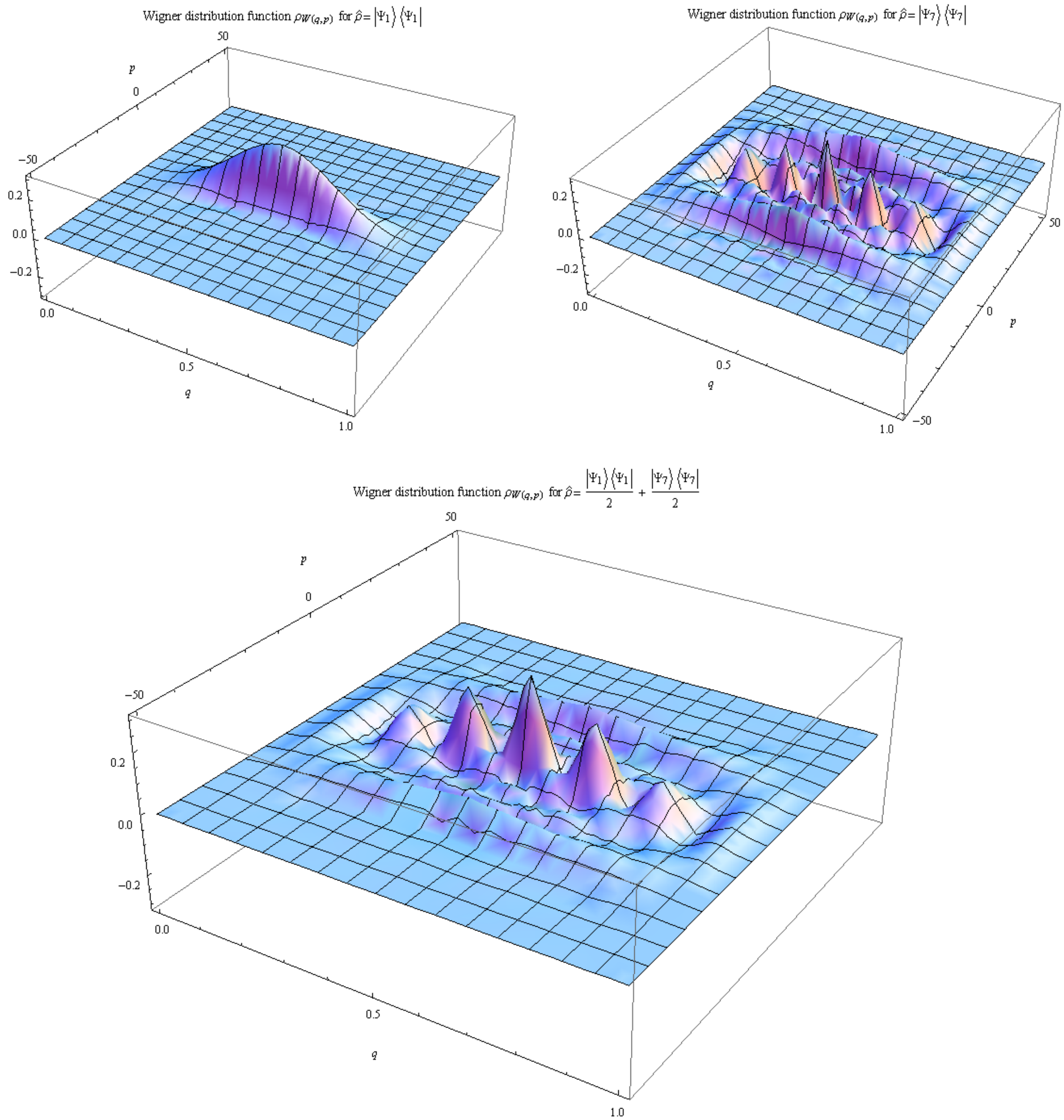

Figure 4: The Wigner distribution function for the pure states with $n = 1$ (top left) and $n = 7$ (top right). They can be combined to find the Wigner distribution function of the mixed state given by (6.21) (bottom). All figures are in the rescaled variables given by (6.15).

6.1.3 Expectation values

In this section we will calculate expectation values of observables making use of the Wigner distribution function. Recall how we calculate expectation values using the Weyl transform and the Wigner distribution with equation (4.27)

$$\langle \hat{A} \rangle = \iint \rho_W(q,p) A_w(q,p) \mathrm{d}q\mathrm{d}p. \tag{6.23}$$

As discussed in section 3 the inverse Weyl transform of polynomials in $\hat{q}$ and $\hat{p}$ are straightforward. As the Hamiltonian in our problem is of the simple form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}), \tag{6.24}$$

we can calculate the inverse Weyl transform by replacing $\hat{p}$ and $\hat{q}$ by respectively p and q. In this section we will calculate the following expectation values and compare them to the results given by the usual wave formulation of quantum mechanics

$$\langle \hat{p} \rangle = \iint \rho_W(q,p) p \mathrm{d}q\mathrm{d}p, \tag{6.25a}$$

$$\langle \hat{q} \rangle = \iint \rho_W(q,p) q \mathrm{d}q\mathrm{d}p, \tag{6.25b}$$

$$\langle \hat{H} \rangle = \iint \rho_W(q,p) \left(\frac{p^2}{2m} + V(q) \right) \mathrm{d}q\mathrm{d}p. \tag{6.25c}$$

We start with the calculation of $\langle \hat{p} \rangle$. We first calculate the expectation value using the wave function given by equation (6.3).

$$\langle \hat{p} \rangle = \int \Psi(q)^* \left(\frac{\hbar}{i} \frac{\partial}{\partial q} \right) \Psi(q) \mathrm{d}q \tag{6.26}$$

$$= \int_0^a \frac{-i\hbar}{n\pi} \sin\left(\frac{2n\pi}{a} q \right) \mathrm{d}q = 0. \tag{6.27}$$

Now we would like to find the same result using the Wigner distribution function. To solve the integral given by (6.25a) we make use of the property that for this specific case the Wigner distribution function is symmetric in the p variable *i.e.*

$$\rho_W^n(q,p) = \rho_W^n(q,-p). \tag{6.28}$$

This can be seen by direct substitution in (6.10). This means that $\rho_W^n(q,p)$ is an even function and thus $\rho_W^n(q,p)p$ is an odd function with respect to the variable p. As the integration of odd functions over symmetric intervals vanish we have

$$\int \rho_W^n(q,p) p \mathrm{d}p = 0, \tag{6.29}$$

and thus $\langle \hat{p} \rangle = 0$. This is the same result we obtained by calculating the expectation value using the usual way.

Similar we now look at the expectation value of $\hat{q}$, again using the well known wave function we have

$$\langle \hat{q} \rangle = \frac{2}{a} \int_0^a q \sin^2\left(\frac{n\pi}{a} q \right) \mathrm{d}q = \frac{1}{2} a. \tag{6.30}$$

If we want to solve this expectation value using Wigner distribution function we need to solve (6.25b)

$$\langle \hat{q} \rangle = \iint \rho_W^n(q,p) q \mathrm{d}q\mathrm{d}p = \int q \left(\int \rho_W^n(q,p) \mathrm{d}p \right) \mathrm{d}q. \tag{6.31}$$

If we make use of (6.20), we find that equation (6.31) becomes the same integral as (6.30) and thus both methods coincide and yield the result

$$\langle \hat{q} \rangle = \frac{1}{2}a. \tag{6.32}$$

Lasty we calculate $\langle \hat{H} \rangle$. We can again make use of the marginals property of the Wigner distribution function

$$\begin{aligned} \langle \hat{H} \rangle &= \iint \rho_W^n(q,p) H(q,p) \mathrm{d}q \mathrm{d}p && (6.33)\\ &= \int_0^a \frac{p^2}{2m} \left(\int_{-\infty}^{\infty} \rho_W^n(q,p) \mathrm{d}q \right) \mathrm{d}p && (6.34)\\ &= \int_0^a \frac{p^2}{2m} \left| \langle \Psi | p \rangle \right|^2 \mathrm{d}p. && (6.35) \end{aligned}$$

This last integral is the same integral we would have obtained by calculating the expectation value using the wave equation in the momentum representation. We thus find again an equivalent result. The calculation of this integral can be calculated with more ease when done in the position representation, we find

$$\begin{aligned} \langle \hat{H} \rangle &= \frac{1}{2m} \int_0^a \Psi(q)^* \left(-\hbar^2 \frac{\partial^2}{\partial q^2} \right) \Psi(q) \mathrm{d}q && (6.36)\\ &= \frac{\hbar^2 n^2 \pi^2}{2ma^2} \int_0^a \Psi(q)^* \Psi(q) \mathrm{d}q && (6.37)\\ &= \frac{\hbar^2 n^2 \pi^2}{2ma^2}. && (6.38) \end{aligned}$$

6.2 Semi classical limit of the infinite potential well

We now want to investigate the semi classical limit. We first discuss the classical situation of a particle with mass m with a given energy E trapped in a box. The particle bounces between the walls with a constant speed given by

$$p_n^2 = 2mE. \tag{6.39}$$

At the boundary the particle undergoes a discontinuous jump in momentum due the collision with the wall. This can be illustrated by a trajectory in phase space shown in figure 5.

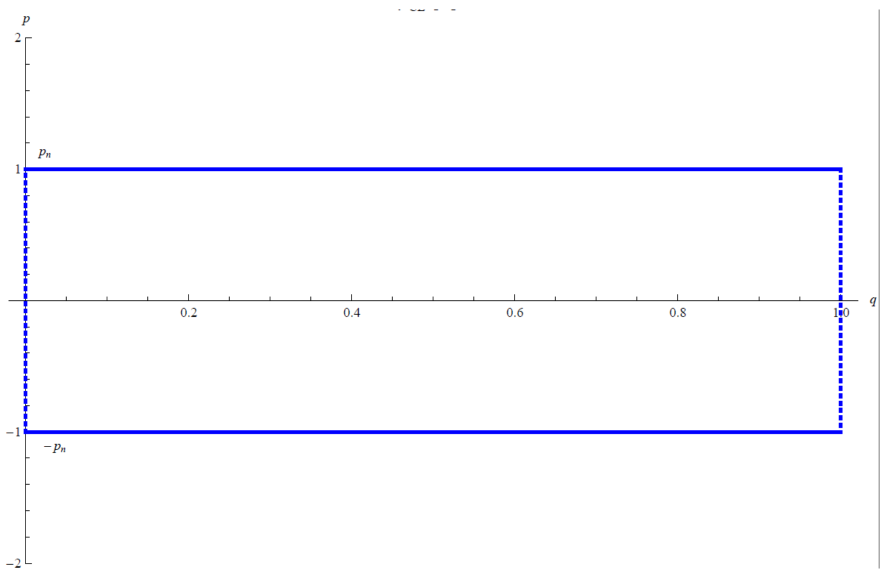

Figure 5: The classical phase space trajectory of a particle in a box.

The corresponding classical probability distribution is then

$$\rho_{Cl}(q,p) = A\delta(E - \tfrac{p^2}{2m}), \quad \text{for } 0 \leq q \leq a. \tag{6.40}$$

In the above equation A is a normalization constant. If we now calculate the marginal equations we find

$$P(q) = \int A\delta(E - \frac{p^2}{2m})\mathrm{d}p = \frac{A}{p_n}. \tag{6.41}$$

And similar for the momentum distribution

$$P(p) = \int_0^a A\delta(E - \frac{p^2}{2m})\mathrm{d}q = aA\delta(E - \frac{p^2}{2m}). \tag{6.42}$$

After normalization we find

$$P(q) = \frac{1}{L}, \tag{6.43a}$$

$$P(p) = \frac{1}{2}(\delta(p + p_n) + \delta(p - p_n)). \tag{6.43b}$$

We can compare these probability distributions to the quantum mechanical analogue for the probability distributions $|\langle q|\Psi\rangle|^2$ and $|\langle p|\Psi\rangle|^2$. In figure 6 we plotted on the left the probability distributions for position and on the right the probability distributions for momentum. The red dotted lines represent the classical probability distribution given by (6.43). We make use of the energy relation (6.2) and setting it equal to the classical energy given by (6.39). This yields in our rescaled variables

$$p'_n = \pm n\pi. \tag{6.44}$$

The blue lines are the quantum probability distributions given by (6.5) and (6.6).

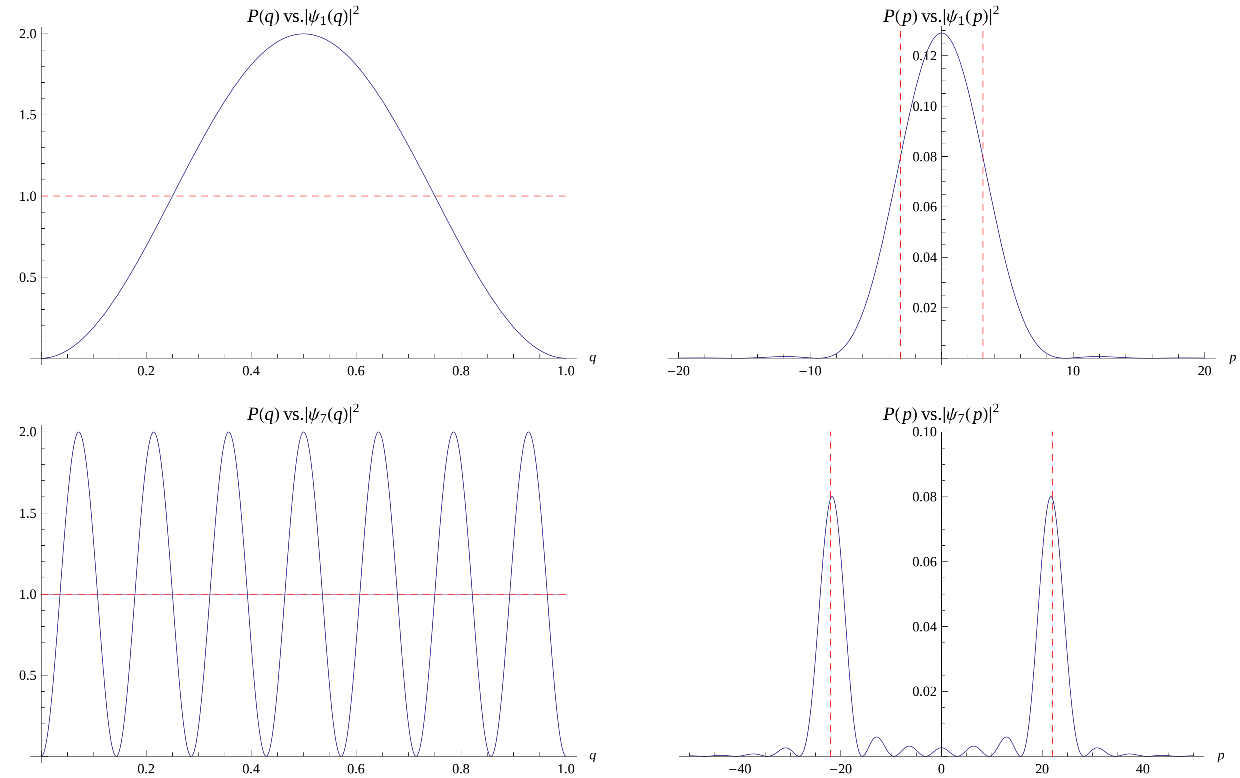

Figure 6: Comparing the classical with the quantum probability distributions for the two different energy eigenstates with $n = 1$ and $n = 7$. We again plotted in our rescaled variables given by (6.15).

The semi classical limit is obtained when we send $\hbar \to 0$. In our rescaled variables we can effectively obtain this effect by looking at large values for n. Recall that the energy is given by (6.2). If we fix the width a, the mass m and the energy E of our system we obtain the following relation

$$E \propto n^2\hbar^2, \qquad\qquad n = 1, 2, 3, \dots, \tag{6.45}$$

from which we conclude that by sending $n \to \infty$ we obtain effectively the effect of $\hbar \to 0$.

This can be seen in figure 6. For large n *i.e* $n = 7$ we see that the (blue) quantum probability distributions start to approximate the (red) classical probability distributions. The quantum position probability distributions describe the probability that a particle in in a given interval. For classical intervals this means that we must average the oscillations which yields for large enough n approximately the classical distribution function. We want to look at the same limit but now for the Wigner distribution function. In figure 7 the Wigner distribution function of a particle in a box is plotted for $n = 7$.

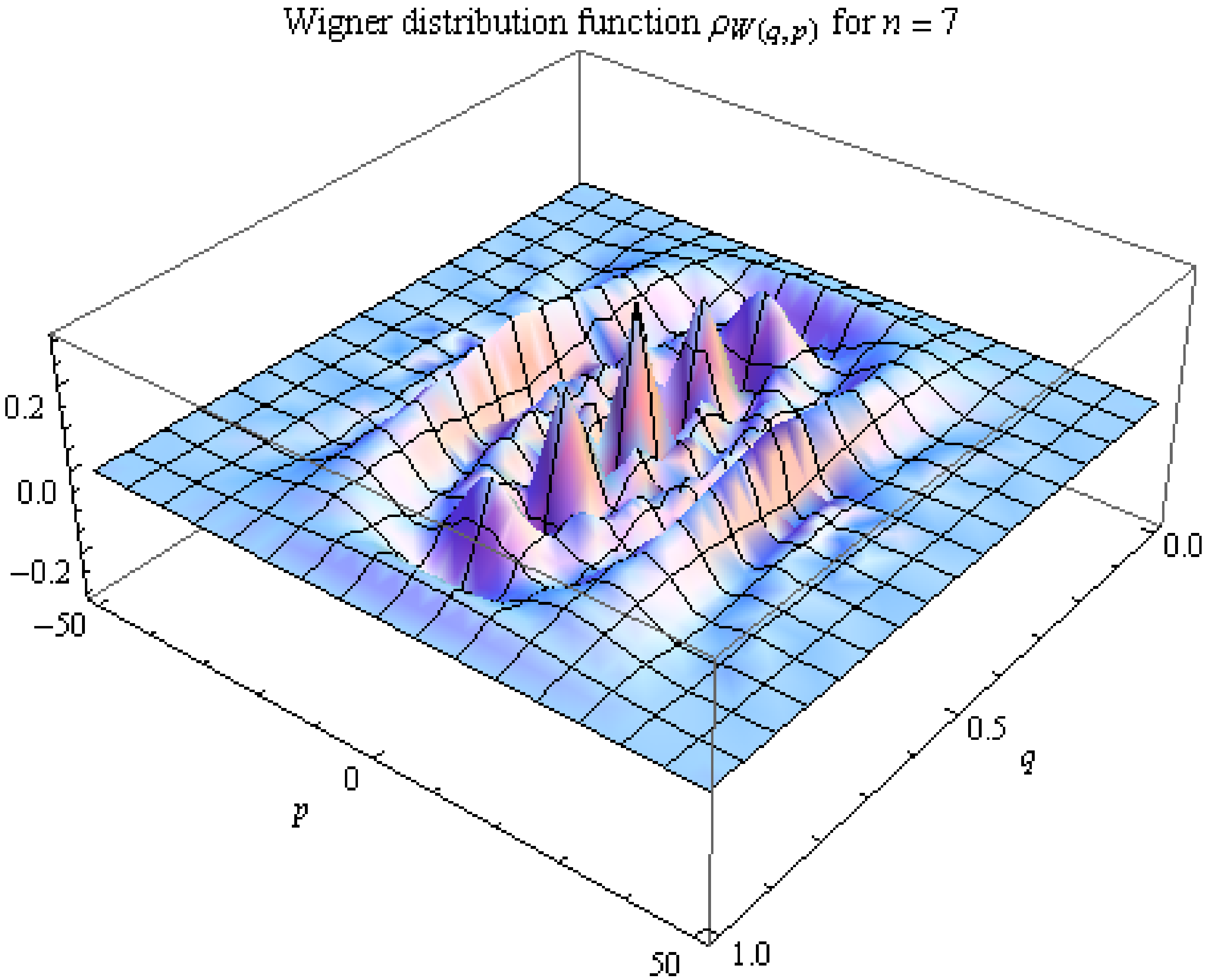

Figure 7: Wigner distribution function of a particle in a box for $n = 7$. We again plotted in our rescaled variables given by (6.15).

The classical equivalent given by (6.40) resembles the phase space trajectory shown in figure 5. There is only probability for at $p = \pm p_n$. The Wigner distribution has these similar probability bumps located at $\pm p_n$, in the rescaled variables given by (6.44). In between these bumps we see allot of oscillations in the Wigner distribution function due to quantum interference. Similar as we argued for the marginal probability distribution functions we classically are interested in intervals of certain size such that we should average over these oscillations. For large n the oscillations in the middle average to zero and we find our classical probability distribution function.

6.3 Husimi distribution of the infinite potential well

In this section we will discuss the Husimi distribution function for the infinite potential well. Recall that we can obtain the Husimi distribution function by a Gaussian smoothing of the Wigner distribution function given by (5.17). For computational reasons we only look at the ground state. In figure 8 the Husimi distribution function is plotted for the ground state with $s = \frac{1}{2}\sqrt{2}a$. The figure is obtained by approximating the domain of the integral in (5.17) by a finite region. we again used the rescaled variables combined with

$$\rho'_H = \hbar \rho_H. \tag{6.46}$$

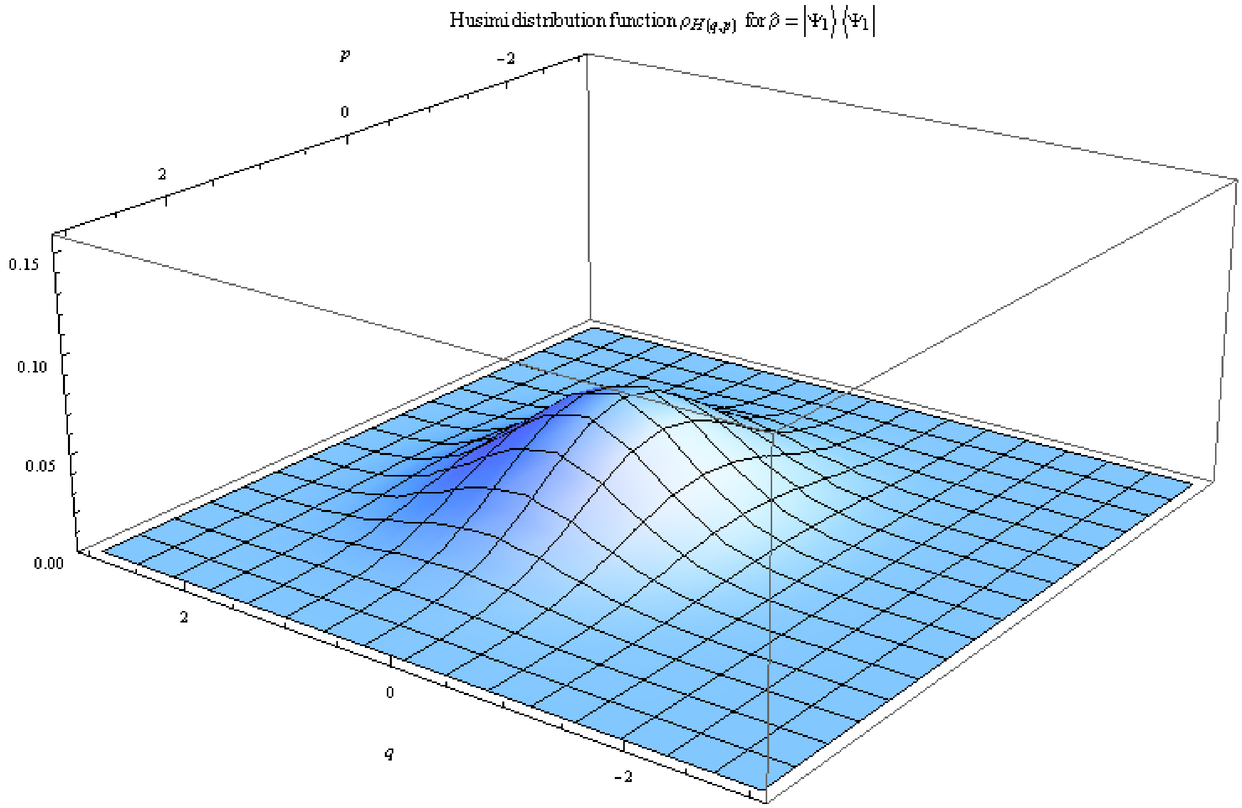

Figure 8: Husimi distribution function of a particle in a box for $n = 1$. We again plotted in our rescaled variables given by (6.15) with (6.46).

For this example we see that the Husimi distribution function is positive bounded by noting that

$$0 < \rho'_H(q,p) \leq \frac{1}{2\pi}. \tag{6.47}$$

The reason why the Husimi distribution function is not a real probability density is because it does not yield the correct marginal distributions given by (4.1). We can easily see that this is indeed not the case in our example. We first note that the Husimi distribution function $\rho_H(q,p)$ does not vanish outside the region of the potential well. Assume for contradiction that the Husimi distribution whould yield the correct marginal distribution functions. Look at a position interval $[a,b]$ outside the potential well. We have that

$$\int_a^b \left(\int \rho_H(q,p) \mathrm{d}p \right) \mathrm{d}q > 0, \tag{6.48}$$

which under the assumption has the interpretation the probability that the particle is in the interval $[a, b]$. However we know from (6.5) that this probability for an interval outside the potential well is zero, which shows the contradiction.

7 Dynamics

We now come to the point where we want to investigate more than just the static behaviour of phase space distributions. We first shortly recall the dynamic equations in classical and in the usual quantum mechanics. Inspired by the description of the dynamics in classical and the usual quantum mechanics, we develop a tool to describe the dynamics for phase space distributions.

7.1 Dynamics in classical mechanics

In the Hamilton mechanics the equations of motion are described by the so called Hamilton equations given by

$$\frac{\mathrm{d}q}{\mathrm{d}t} = +\frac{\partial H}{\partial p}, \tag{7.1a}$$

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H}{\partial q}. \tag{7.1b}$$

Where $H(q, p, t)$ is the Hamiltonian of the system given by the total energy.

Definition 7.1 (Hamiltonian flow)**.** *The Hamiltonian flow is the function $\Phi_t : \mathcal{P} \times \mathbb{R} \to \mathcal{P}$ which time evolves the initial state (q_0, p_0) according to the Hamilton equations* (7.1) *[23]*

$$\Phi_t(q_0, p_0) = (q(t), p(t)), \qquad \textit{with } (q(0), p(0) = (q_0, p_0). \tag{7.2}$$

The flow has the following properties [13]

$$\Phi_{t_1} \circ \Phi_{t_2} = \Phi_{t_1+t_2}, \tag{7.3}$$

$$\Phi_t \circ \Phi_{-t} = id, \tag{7.4}$$

$$\Phi_0 = id. \tag{7.5}$$

Here id denotes the identity map on phase space.

In classical mechanics one can put the time dependence in the states as well as in the observables similar to the Schrödinger and the Heisenberg picture in quantum mechanics . Recall that in classical mechanics observables are given by continuous functions acting on the state space. We define the time evolved observable f by composing it with the flow.

$$f(q_0, p_0, t) = f \circ \Phi_t(q_0, p_0). \tag{7.6}$$

We will restrict to time independent observables f which can be made into time dependent observables $f(t)$ by (7.6). In this picture with time dependent observables $f(t)$ we have time independent classical states.

Definition 7.2 (Poisson bracket)**.** *The Poisson bracket $\{\cdot, \cdot\}_{PB}$ is defined as the bilinear map $C^\infty(\mathcal{P} \times \mathbb{R}) \times C^\infty(\mathcal{P} \times \mathbb{R}) \to C^\infty(\mathcal{P} \times \mathbb{R})$,*

$$\{f, g\}_{PB} = \frac{\partial f}{\partial q}\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial q}, \tag{7.7}$$

where the two functions $f(q, p, t)$ and $g(q, p, t)$ are both in $C^\infty(\mathcal{P} \times \mathbb{R})$.

We can express the time evolution of classical observables $f(q, p, t) \in C^\infty(\mathcal{P} \times \mathbb{R})$ in terms of the Poisson bracket.

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} f(q, p, t) &= \frac{\mathrm{d}}{\mathrm{d}t} f(q(t), p(t)) = \frac{\partial f(q, p, t)}{\partial q}\frac{\mathrm{d}q}{\mathrm{d}t} + \frac{\partial f(q, p, t)}{\partial p}\frac{\mathrm{d}p}{\mathrm{d}t} \\ &= \frac{\partial f(q, p, t)}{\partial q}\frac{\mathrm{d}H(q, p, t)}{\mathrm{d}p} - \frac{\partial f(q, p, t)}{\partial p}\frac{\mathrm{d}H(q, p, t)}{\mathrm{d}q} \\ &= \{f(q, p, t), H(q, p, t)\}_{PB}. \end{aligned} \tag{7.8}$$

We made use of the Hamilton equations given by (7.1) to get from the first to the second line. We conclude classically the time evolution of any differentiable function defined on phase space is given by

$$\frac{\mathrm{d}}{\mathrm{d}t} f(q,p,t) = \{f, H\}_{PB}. \tag{7.9}$$

Example 7.1 (Classical conserved energy)**.** We can as an example calculate the time evolution of the Hamiltonian observable which describes the total energy in the system.

$$\frac{\mathrm{d}}{\mathrm{d}t} H(q,p,t) = \{H(q,p,t), H(q,p,t)\}_{PB} = 0. \tag{7.10}$$

We conclude that the $H(q,p,t)$ is a conserved quantity.

7.2 Dynamics in quantum mechanics

We again want to work in the Heisenberg picture where all the dynamics is put inside the operators instead of the state. We will only look at time independent Hamiltonian operators. In the general Schrödinger picture the expectation value of any operator $\hat{A}$ in the pure state $\Psi(t)$ is given by

$$\langle \hat{A} \rangle (t) = \langle \Psi(t) | \hat{A} | \Psi(t) \rangle . \tag{7.11}$$

All the time evolution is put inside the state $\Psi(t)$ which is given by [7]

$$|\Psi(t)\rangle = e^{-\frac{i\hat{H}t}{\hbar}} |\Psi(0)\rangle . \tag{7.12}$$

Where $\hat{H}$ is the Hamiltonian operator of the system. Using this explicit relation we can rewrite (7.11) as

$$\langle \hat{A} \rangle (t) = \langle \Psi(0) | e^{\frac{i\hat{H}t}{\hbar}} \hat{A} e^{-\frac{i\hat{H}t}{\hbar}} | \Psi(0) \rangle . \tag{7.13}$$

We now define Heisenberg operators denoted by $\hat{A}_H$ in terms of the schrödinger operators denoted by $\hat{A}_S$ as

$$\hat{A}_H(t) = e^{\frac{i\hat{H}t}{\hbar}} \hat{A}_S e^{-\frac{i\hat{H}t}{\hbar}} . \tag{7.14}$$

Similar as in the classical case we can now calculate the time evolution of these Heisenberg operators. We again assume static observables which means $\frac{\partial \hat{A}_S}{\partial t} = 0$. From now on we will explicitly denote the time dependence t for Heisenberg operators and suppress the subscripts S and H for the operators.

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \hat{A}(t) &= \frac{i}{\hbar} \hat{H} e^{\frac{i\hat{H}t}{\hbar}} \hat{A} e^{-\frac{i\hat{H}t}{\hbar}} - e^{\frac{i\hat{H}t}{\hbar}} \hat{A} \frac{i}{\hbar} \hat{H} e^{-\frac{i\hat{H}t}{\hbar}} \\ &= \frac{i}{\hbar} e^{\frac{i\hat{H}t}{\hbar}} (\hat{H}\hat{A} - \hat{A}\hat{H}) e^{-\frac{i\hat{H}t}{\hbar}} \\ &= \frac{i}{\hbar} [\hat{H}, \hat{A}(t)]. \end{aligned} \tag{7.15}$$

Where in the last step we used the fact that $\hat{H}$ commutes with $e^{\frac{i\hat{H}t}{\hbar}}$ to find our wanted result

$$\frac{\mathrm{d}}{\mathrm{d}t} \hat{A}(t) = \frac{i}{\hbar} [\hat{H}, \hat{A}(t)]. \tag{7.16}$$

This expression is similar to what we found in the classical case given by (7.9). It appears that in quantum mechanics the Poisson bracket up to a factor is replaced with the commutator.

Example 7.2 (Quantum mechanical conserved energy)**.** Just as our example in the classical case we can also calculate the time dependence of the Hamiltonian operator which is given by

$$\frac{\mathrm{d}}{\mathrm{d}t} \hat{H}(t) = \frac{i}{\hbar} [\hat{H}, \hat{H}(t)] = 0.$$

We find the same conclusion, the total energy of the system is a conserved quantity.

7.3 Moyal product

In the previous sections we discussed how classically the time evolution is described on phase space. We also discussed how quantum mechanically the time evolution is described for operators in Hilbert space. Our goal is now to combine these two and find a quantum mechanical description for the time evolution of functions on phase space. For quantum mechanics defined on phase space to coincide with regular quantum mechanics the time evolution of functions should be equivalent to the corresponding time evolution of operators in Hilbert space. Also for classical mechanics to be a limiting case of quantum mechanics we require that the time evolution in its classical limit should reduce to the known classical time evolution.

We will look at the time evolution of the phase space function A. Our goal is to find the one parameter family of functions on phase space $A(t)$ which corresponds to the operator $\hat{A}(t)$ *i.e.*[13]

$$\Phi[A(t)] = e^{+\frac{i\Phi[H]t}{\hbar}} \Phi[A] e^{-\frac{i\Phi[H]t}{\hbar}}. \tag{7.17}$$

Here $\Phi[H]$ denotes the Weyl transform of the Weyl symbol of the Hamiltonian operator. Taking the inverse Weyl transform we find while making use of (3.11)

$$A(t) = (e^{+\frac{iHt}{\hbar}}) \star_M A \star_M (e^{-\frac{iHt}{\hbar}}). \tag{7.18}$$

The exponents in this equation should be read as their Taylor expansion with the Moyal product instead of the normal product *i.e.*

$$H^2 = H \star_M H. \tag{7.19}$$

Similar to the calculation for the time evolution of Heisenberg operators in (7.16) we now take the derivative to the parameter t to find

$$\frac{\mathrm{d}}{\mathrm{d}t} A(t) = \{A(t), H\}_M. \tag{7.20}$$

The factor $\frac{1}{i\hbar}$ we had in front of the commutator in (7.16) is now put inside the definition of the Moyal bracket (3.13).

The following diagram commutes

$$\begin{tikzcd}
A(t_0) \arrow[r, shift left, "\Phi"'] \arrow[d, "\frac{\mathrm{d}}{\mathrm{d}t} A = \{A, H\}_M"'] & \hat{A}(t_0) \arrow[l, shift left, "\Phi^{-1}"'] \arrow[d, "\frac{\mathrm{d}}{\mathrm{d}t} \hat{A} = \frac{1}{i\hbar}[\hat{A}, \hat{H}]"] \\
A(t_1) \arrow[r, shift left, "\Phi"] & \hat{A}(t_1) \arrow[l, shift left, "\Phi^{-1}"]
\end{tikzcd}$$

Figure 9: Time evolution of observables in phase space and in Hilbert space.

We need to solve the differential equation (7.20) with initial condition $A(t_0) = A$ to find the time evolution of the symbol of $\hat{A}$. To study the dynamics we need to take a closer look at the Moyal bracket. The explicit form of the Moyal bracket is derived in appendix A and given by

$$\{A(q,p), B(q,p)\}_M = \frac{2}{\hbar} A(q,p) \sin\left(\frac{\hbar}{2}(\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q})\right) B(q,p). \tag{7.21}$$

If we write the first term of the Moyal product we find

$$\{A(q,p), B(q,p)\}_M = A(q,p)(\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q})B(q,p) + \mathcal{O}(\hbar^2), \tag{7.22}$$

which is exactly the Poisson bracket plus higher order terms

$$\{A(q,p), B(q,p)\}_M = \{A(q,p), B(q,p)\}_{PB} + \mathcal{O}(\hbar^2). \tag{7.23}$$

This result suggest that the dynamics of a quantum system can be described by the classical dynamics perturbed with quantum terms. For this reason if one is interested in the semi classical limit the phase space formulation is often studied. In the special case when at least one of $A(q,p)$ or $B(q,p)$ is a second order polynomial the Moyal product becomes exactly the Poisson bracket *i.e.*

$$\{A(q,p), B(q,p)\}_M = \{A(q,p), B(q,p)\}_{PB}. \tag{7.24}$$

This means that for systems whose corresponding Hamiltonian is at most a second order polynomial have the dynamics described by the Poisson bracket and thus are equivalent to the classical dynamics.

Theorem 7.1 (Exact Egorov)**.** *Assume the classical Hamiltonian $H(q,p)$ is a polynomial of order less than or equal to two with real valued coefficients. For $T > 0$ let Φ_t be the Hamiltonian flow associated to $H(q,p)$ for all $t \in [-T,T]$ according to equation (7.2). Let $\hat{H}$ denote the Weyl transform of the symbol $H(q,p)$. Then*

$$\hat{U} = e^{-\frac{i}{\hbar}\hat{H}}, \tag{7.25}$$

is unitary, and for every real valued classical observable $A \in S^m(\mathcal{P})$ we have that

$$\hat{A}(t) = e^{\frac{i}{\hbar}\hat{H}t}\hat{A}e^{-\frac{i}{\hbar}\hat{H}t} = \widehat{A \circ \Phi_t}. \tag{7.26}$$

Where again the hat denotes the Weyl transform and $\widehat{A \circ \Phi_t} \in S^m(\mathcal{P})$. In this theorem we work in the Heisenberg picture. In figure 9, for these systems we can replace the Moyal bracket by the classical Poisson bracket.

The reason this theorem goes by the name the exact Egorov theorem is because there is a more general class of Hamiltonian functions for which equation (7.26) holds in an approximate sense, that is the error is of order $\mathcal{O}(\hbar^2)$. The proof of the more general theorem can be found in [9]. The higher order terms vanish only if the conditions of theorem 7.1 are satisfied [13].

Up till this point we have been working in the Heisenberg picture of quantum mechanics. In the Heisenberg picture the states and thus the density operator has no time evolution. If we want to determine the time evolution of the Wigner distribution function we have to work in the Schrödinger picture. The time evolution of the density operator follows directly from (7.12)

$$\hat{\rho}(t) = e^{-\frac{i}{\hbar}\hat{H}t}\hat{A}e^{+\frac{i}{\hbar}\hat{H}t}, \tag{7.27}$$

note the sign difference in the exponential compared to observables. When we want to calculate the time evolution of the Wigner distribution we can still make use of the Egorov theorem by composing with Φ_{-t}.

Example 7.3 (Harmonic oscillator)**.** The well known problem of the harmonic oscillator has the classical Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2. \tag{7.28}$$

This Hamiltonian satisfies the conditions of theorem 7.1.

The Hamiltonian flow of the harmonic oscillator is given by

$$\Phi_t(q_0,p_0) = \left(q_0\cos(\omega t) + \frac{p_0}{m\omega}\sin(\omega t), -m\omega q_0\sin(\omega t) + p_0\cos(\omega t)\right). \tag{7.29}$$

Now let $\rho_W(q_0,p_0)$ denote the Wigner distribution function at time $t=0$ at position (q_0,p_0). We can now calculate the Wigner distribution function at a given time t by

$$\rho_W(q,p,t) = (\rho_W \circ \Phi_{-t})(q,p) = \rho_W\left(q\cos(\omega t) - \frac{p}{m\omega}\sin(\omega t), m\omega q\sin(\omega t) + p\cos(\omega t)\right). \tag{7.30}$$

8 Conclusion

The presented phase space formulation of quantum mechanics is a complete and equivalent formulation of quantum mechanics. We have seen that there exist many non equivalent phase space distribution functions describing quantum mechanics. We however can not speak of a real probability density due the quantum behaviour. The Wigner distribution function has the property that it in general attains negative values. The Husimi distribution is a positive distribution function but lacks the property of yielding the correct marginal distributions. There does not exist a phase space distribution which is bilinear in the wave function and satisfies both these conditions.

An advantage of the phase space formulation is that it closely related to how we define classical mechanics. For this reason it can be used to study the semi classical limit. The time evolution in the phase space formulation consist of the classical time evolution perturbed with higher order quantum terms. For certain systems these quantum interference terms vanish and the time evolution of the Wigner distribution function becomes the same as the classical time evolution. This can be extended to a larger class of systems for which the dynamics becomes classical in the classical limit when $\hbar$ goes to zero.

An other advantage of the phase space formulation can be found in studying mixed states. The Wigner distribution function of mixed states can be described as a linear combination of the Wigner distribution functions of pure states. The Schrödinger equation is written in terms of pure states and does initially not describe time evolution for mixed states. However the Wigner distribution function in the phase space formalism can be used to study the time evolution of mixed states.

One might ask if we then should choose the phase space formulation over the usual wave formalism of quantum mechanics? The answer depends on the both the system and the objective of the problem. The Schrödinger equation is ideal for finding exact or approximate solutions. However certain systems let them describe nicely in the phase space formalism. The Wigner distribution function has found many applications one of which is the study of collisions. The Husimi distribution function finds many applications in quantum optics [6]. Also if one is interested in studying the classical limit one might favour the phase space formulation.

Appendices

A Moyal product and Moyal Bracket

In this section we will derive the Moyal product given by (3.12). We follow the original proof by Groenewold [3].

Recall the Moyal product is the product defined between phase space functions such that (3.11) holds

$$\Phi[A(q,p) \star_M B(q,p)] = \Phi[A(q,p)] \cdot \Phi[B(q,p)]. \tag{A.1}$$

We calculate the right hand side of this equation by using the Weyl transform (3.9)

$$\begin{aligned}\hat{A}\hat{B} = \left(\frac{1}{2\hbar\pi}\right)^4 \iint \cdots \iint A(q,p) e^{\frac{i}{\hbar}(y(\hat{q}-q)+x(\hat{p}-p))} \\ \cdot B(q',p') e^{\frac{i}{\hbar}\left(y'(\hat{q}-q')+x'(\hat{p}-p')\right)} \mathrm{d}q \mathrm{d}p \mathrm{d}y \mathrm{d}x \mathrm{d}q' \mathrm{d}p' \mathrm{d}y' \mathrm{d}x'.\end{aligned} \tag{A.2}$$

We can rewrite this equation using the Baker-Hausdorff identity (2.25)

$$\begin{aligned}\hat{A}\hat{B} = \left(\frac{1}{2\hbar\pi}\right)^4 \iint \cdots \iint A(q,p) e^{\frac{i}{\hbar}(\hat{q}(y+y')+\hat{p}(x+x'))} e^{\frac{i}{2\hbar}(xy'-yx')} \\ \cdot e^{\frac{-i}{\hbar}(yq+y'q'+xp+x'p')} B(q',p') \mathrm{d}q \mathrm{d}p \mathrm{d}y \mathrm{d}x \mathrm{d}q' \mathrm{d}p' \mathrm{d}y' \mathrm{d}x'.\end{aligned} \tag{A.3}$$

We now make use of the following change of variables

$$\begin{array}{llll} \xi = x + x', & \eta = y + y', & \tau = \frac{q+q'}{2}, & \sigma = \frac{p+p'}{2}, \\ \xi' = \frac{x-x'}{2}, & \eta' = \frac{y-y'}{2}, & \tau' = q - q' & \sigma' = p - p'. \end{array} \tag{A.4}$$

Using this change of variables we find

$$\begin{aligned}\hat{A}\hat{B} = \left(\frac{1}{2\hbar\pi}\right)^4 \iint \cdots \iint A(\tau + \frac{1}{2}\tau', \sigma + \frac{1}{2}\sigma') e^{\frac{i}{\hbar}(\hat{q}\eta+\hat{p}\xi)} e^{\frac{i}{2\hbar}(-\xi\eta'+\eta\xi')} \\ \cdot e^{\frac{-i}{\hbar}(\xi\sigma+\xi'\sigma'+\eta\tau+\eta'\tau')} B(\tau - \frac{1}{2}\tau', \sigma - \frac{1}{2}\sigma') \mathrm{d}\sigma \mathrm{d}\tau \mathrm{d}\xi \mathrm{d}\eta \mathrm{d}\sigma' \mathrm{d}\tau' \mathrm{d}\xi' \mathrm{d}\eta'.\end{aligned} \tag{A.5}$$

Where made use of the Jacobian rule for the change of variables

$$\mathrm{d}\eta \mathrm{d}\eta' = \left|\frac{\partial(\eta,\eta')}{\partial(y,y')}\right| \mathrm{d}y \mathrm{d}y' = \mathrm{d}y \mathrm{d}y'. \tag{A.6}$$

In this equation $\frac{\partial(\eta,\eta')}{\partial(y,y')}$ denotes the Jacobian of the change of variables which is in absolute value 1 in our case for all changed variables.

If we now perform the integration over $\mathrm{d}\xi'\mathrm{d}\eta'$ we pick up the factor

$$\left(\frac{1}{2\hbar\pi}\right)^2 \delta(\tau' + \frac{1}{2}\xi)\delta(\frac{1}{2}\eta - \sigma').$$

Integration over $\mathrm{d}\tau'\mathrm{d}\sigma'$ gives us

$$\hat{A}\hat{B} = \left(\frac{1}{2\hbar\pi}\right)^2 \iiiint A(\tau - \frac{1}{4}\xi, \sigma + \frac{1}{4}\eta) B(\tau + \frac{1}{4}\xi, \sigma - \frac{1}{4}\eta) e^{\frac{i}{\hbar}(\hat{q}\eta+\hat{p}\xi)} e^{\frac{-i}{\hbar}(\xi\sigma+\eta\tau)} \mathrm{d}\sigma \mathrm{d}\tau \mathrm{d}\xi \mathrm{d}\eta. \tag{A.7}$$

We now make use of the Taylor expansion of $A(q,p)$ around τ and σ given by

$$A(q,p) = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{(q-\tau)^n(p-\sigma)^m}{n!\,m!} \frac{\partial^{(n+m)}A(q,p)}{\partial q^n \partial p^m}|_{(q,p)=(\tau,\sigma)}. \tag{A.8}$$

Substituting $(q,p) = (\tau - \frac{1}{4}\xi, \sigma + \frac{1}{4}\eta)$ and making use of the Taylor series for e^x we find,

$$A(\tau - \frac{1}{4}\xi, \sigma + \frac{1}{4}\eta) = e^{\frac{1}{4}(\xi\frac{\partial}{\partial q} - \eta\frac{\partial}{\partial p})} A(q,p)|_{(q,p)=(\tau,\sigma)}. \tag{A.9}$$

A similar result holds for $B(\tau + \frac{1}{4}\xi, \sigma - \frac{1}{4}\eta)$. Using the Taylor series we rewrite (A.9) as

$$\begin{aligned}\hat{A}\hat{B} = \left(\frac{1}{2\hbar\pi}\right)^2 \iiiint e^{\frac{i}{\hbar}(\hat{q}\eta + \hat{p}\xi)} e^{\frac{-i}{\hbar}(\xi\sigma + \eta\tau)}.\\ \left(e^{\frac{1}{4}(\xi\frac{\partial}{\partial q} - \eta\frac{\partial}{\partial p})} A(q,p)|_{(q,p)=(\tau,\sigma)}\right) \left(e^{\frac{-1}{4}(\xi\frac{\partial}{\partial q} - \eta\frac{\partial}{\partial p})} B(q,p)|_{(q,p)=(\tau,\sigma)}\right) \mathrm{d}\sigma\mathrm{d}\tau\mathrm{d}\xi\mathrm{d}\eta.\end{aligned} \tag{A.10}$$

If we now rename our variables according to

$$\xi \leftrightarrow x, \qquad \eta \leftrightarrow y, \qquad \tau \leftrightarrow q, \qquad \sigma \leftrightarrow p. \tag{A.11}$$

Partial integration yields us

$$\begin{aligned}\hat{A}\hat{B} = \left(\frac{1}{2\hbar\pi}\right)^2 \iiiint e^{\frac{i}{\hbar}(y(\hat{q}-q) + x(\hat{p}-p))}.\\ \left(A(q,p)\exp\left(i\frac{\hbar}{2}(\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q})\right) B(q,p)\right)\mathrm{d}q\mathrm{d}p\mathrm{d}y\mathrm{d}x.\end{aligned} \tag{A.12}$$

We will show this partial integration explicitly up to the first order terms. We will not go into detail for the higher order terms as the calculation becomes very involved.

The zeroth order term in equation (A.10) and (A.12) are the same. So what is left to check are the first order terms. We will work backwards starting from (A.12). The integral in which we are interested are the q and p integrals. The first order terms leaving the x and y integrals out of this discussion become

$$\iint e^{-\frac{i}{\hbar}(yq+xp)} A(q,p)\left(\frac{i\hbar}{4}(\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q} + \overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q})\right) B(q,p)\mathrm{d}q\mathrm{d}p. \tag{A.13}$$

Here we split the equation in four terms which we want to partial integrate differently. Let us look at one such term. We partial integrate with respect to q to get rid of the $\overleftarrow{\partial_q}$ derivative, making use of the chain rule we find

$$\iint e^{-\frac{i}{\hbar}(yq+xp)} A(q,p)\left(\frac{i\hbar}{4}(\overleftarrow{\partial_q}\overrightarrow{\partial_p})\right) B(q,p)\mathrm{d}q\mathrm{d}p = \iint e^{-\frac{i}{\hbar}(yq+xp)} A(q,p)\left(\frac{y}{4}\overrightarrow{\partial_p} - \frac{i\hbar}{4}\overrightarrow{\partial_{qp}}\right) B(q,p)\mathrm{d}q\mathrm{d}p. \tag{A.14}$$

The second term in this expression will get canceled if we do the same trick of partial integration with respect to p to the fourth term in equation (A.13). We find that after partial integration of (A.13) can be written as

$$\iint e^{-\frac{i}{\hbar}(yq+xp)} A(q,p)\left(\frac{1}{4}(x\overleftarrow{\partial_q} - y\overleftarrow{\partial_p} - x\overrightarrow{\partial_q} + y\overrightarrow{\partial_p})\right) B(q,p)\mathrm{d}q\mathrm{d}p. \tag{A.15}$$

Which is precisely the first order term of (A.10) after the change of variables.

Comparing equation (A.12) with the Weyl transform (3.9) and (A.1) we conclude that the Moyal product is given by,

$$A(q,p) \star_M B(q,p) = A(q,p) \exp\left(i\frac{\hbar}{2}(\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q}) \right) B(q,p). \tag{A.16}$$

Making use of the Moyal product we can now give a representation for the Moyal bracket defined by (3.13). If we make use of Euler's identity for the sine we directly find (7.21)

$$\{A(q,p), B(q,p)\}_M = \frac{2}{\hbar} A(q,p) \sin\left(\frac{\hbar}{2}(\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q}) \right) B(q,p). \tag{A.17}$$

B Wigner function of the infinite well

In this section we will derive the Wigner distribution of the n^{th} energy eigenstate of the infinite potential well given by equation (6.11). We start with the definition of the Wigner distribution function (6.10)

$$\begin{aligned}\rho_W^n(q,p) =& \frac{1}{\pi\hbar}\int_{-q}^{q}\frac{2}{a}\sin\left(\frac{n\pi}{a}(q+y)\right)\cdot\sin\left(\frac{n\pi}{a}(q-y)\right)e^{-2i\frac{py}{\hbar}}\,\mathrm{d}y \\ =& \left(\frac{2}{\pi\hbar a}\right)\left(\frac{\sin\left(2q(\frac{p}{\hbar}-\frac{n\pi}{a})\right)}{4(\frac{p}{\hbar}-\frac{n\pi}{a})}+\frac{\sin\left(2q(\frac{p}{\hbar}+\frac{n\pi}{a})\right)}{4(\frac{p}{\hbar}+\frac{n\pi}{a})}-\cos\left(\frac{2n\pi q}{a}\right)\frac{\sin\left(\frac{2pq}{\hbar}\right)}{\frac{2p}{\hbar}}\right).\end{aligned} \tag{B.1}$$

The first step is by using the trigonometric identity for the product of sine functions

$$\sin\left(\frac{A+B}{2}\right)\sin\left(\frac{A-B}{2}\right)=\frac{1}{2}\left(\cos B-\cos A\right). \tag{B.2}$$

Using equation (B.2) with $A=\frac{2n\pi}{a}q$ and $B=\frac{2n\pi}{a}y$ we find

$$\rho_W^n(q,p)=\frac{1}{a\pi\hbar}\int_{-q}^{q}\left(\cos(\frac{2n\pi}{a}y)-\cos(\frac{2n\pi}{a}q)\right)e^{-2i\frac{py}{\hbar}}\,\mathrm{d}y. \tag{B.3}$$

We will split this integral into two integrals I_1 and I_2 and solve them separately

$$I_1=\int_{-q}^{q}\cos(\frac{2n\pi}{a}y)e^{-2i\frac{py}{\hbar}}\,\mathrm{d}y, \tag{B.4a}$$

$$I_2=\int_{-q}^{q}\cos(\frac{2n\pi}{a}q)e^{-2i\frac{py}{\hbar}}\,\mathrm{d}y. \tag{B.4b}$$

We will start with the easier integral I_2 as it has only y dependence in the exponent

$$I_2=\int_{-q}^{q}\cos(\frac{2n\pi}{a}q)e^{-2i\frac{py}{\hbar}}\,\mathrm{d}y \tag{B.5}$$

$$=\cos(\frac{2n\pi}{a}q)[-\frac{1}{2i\frac{p}{\hbar}}e^{-2i\frac{py}{\hbar}}]_{-q}^{q} \tag{B.6}$$

$$=2\cos(\frac{2n\pi}{a}q)\sin\frac{2pq}{\hbar}. \tag{B.7}$$

To solve I_1 we make use of the standard integral [24]

$$\int e^{bu}\cos cu\mathrm{d}u=\frac{e^{bu}}{c^2+b^2}\left(b\cos cu+a\sin cu\right)+C. \tag{B.8}$$

In the situation of I_1 this is $c=\frac{2n\pi}{a}$ and $b=-2i\frac{p}{\hbar}$. For now we will stick to the notation of the standard integral. Making use of the standard integral and applying the limits we find the following result

$$I_1=\frac{1}{c^+b^2}\left(c(e^{bq}+e^{-bq})\sin(cq)+b(e^{bq}-e^{-bq})\cos(cq)\right) \tag{B.9}$$

$$=\frac{2}{c^-d^2}\left(c\cos(dq)\sin(cq)-d\sin(dq)\cos(cq)\right). \tag{B.10}$$

Where defined the new constant d by $d=Im(b)$. With the help of basic geometric identities we can rewrite (B.10) in a much nicer way

$$I_1=\frac{\sin(c+d)q}{c+d}+\frac{\sin(c-b)q}{c-b}.$$

Substituting the values for c and d we find

$$I_1 = \frac{\sin\left(2q(\frac{p}{\hbar} - \frac{n\pi}{a})\right)}{2(\frac{p}{\hbar} - \frac{n\pi}{a})} + \frac{\sin\left(2q(\frac{p}{\hbar} + \frac{n\pi}{a})\right)}{2(\frac{p}{\hbar} + \frac{n\pi}{a})}. \tag{B.11}$$

Combining all results from above we find our final result

$$\begin{aligned} \rho_W^n(q,p) &= \frac{1}{a\pi\hbar}(I_1 - I_2), \\ &= \left(\frac{2}{\pi\hbar a}\right)\left(\frac{\sin\left(2q(\frac{p}{\hbar} - \frac{n\pi}{a})\right)}{4(\frac{p}{\hbar} - \frac{n\pi}{a})} + \frac{\sin\left(2q(\frac{p}{\hbar} + \frac{n\pi}{a})\right)}{4(\frac{p}{\hbar} + \frac{n\pi}{a})} - \cos\left(\frac{2n\pi q}{a}\right)\frac{\sin\left(\frac{2pq}{\hbar}\right)}{\frac{2p}{\hbar}}\right). \end{aligned} \tag{B.12}$$

Note that this expression is symmetric around $p = 0$. The Wigner distribution function defined on the whole interval $q \in [0, a]$ is also symmetric around $q = \frac{1}{2}a$. This follows directly from how we defined the Wigner distribution function for $q \in [\frac{1}{2}a, a]$

$$\rho_W^n(q,p) = \rho_W^n(a - q, p). \tag{B.13}$$

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