Non-positivity of Groenewold operators

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Abstract

A central feature in the Hilbert space formulation of classical mechanics is the quantisation of classical Liouville densities, leading to what may be termed term Groenewold operators. We investigate the spectra of the Groenewold operators that correspond to Gaussian and to certain uniform Liouville densities. We show that when the classical coordinate-momentum uncertainty product falls below Heisenberg’s limit, the Groenewold operators in the Gaussian case develop negative eigenvalues and eigenvalues larger than 1. However, in the uniform case, negative eigenvalues are shown to persist for arbitrarily large values of the classical uncertainty product.

1 Introduction

The phase space formulation of quantum mechanics has its origins in the work of Weyl [1] and Wigner [2] more than 70 years ago. In this formulation, quantum observables are represented by phase space functions and quantum states by quasi-density (Wigner) functions that evolve in time according to a deformation of the classical Liouville equation. Although many calculations are more difficult to perform in the phase space context, this formulation has the distinct advantage of the common language of phase space for the purpose of comparing classical and quantum dynamics. Indeed, it was for such a purpose (the calculation of quantum corrections to thermodynamic quantities) that Wigner first introduced his now famous function.

This begs the following question: if quantum mechanics can be described in the classical setting of phase space, can classical mechanics be described in the quantum setting of Hilbert space? In fact, it was already recognised by Groenewold [3] nearly 60 years ago that this is possible and, after related work in the interim [4, 5, 6, 7, 8], it has recently been made explicit [9]. The key to understanding this is to recognise the unitarity, and hence the invertibility, of the Weyl-Wigner transform [10, 11], which maps quantum operators into phase space functions.
The inverse transform is Weyl’s quantisation map, which transforms classical functions (observables) into linear operators on Hilbert space. Just as the quantum density operator is mapped into a quasi-probability function on phase space (a Wigner function) by the Weyl-Wigner transform, so a classical Liouville density function on phase space is mapped by the inverse transform into a quasi-density operator on Hilbert space (which we suggest to call a Groenewold operator). Just as a Wigner function is normalised on all of phase space, but is not in general a non-negative definite function, so a Groenewold operator has unit trace, but is not in general a non-negative definite operator. Just as quantum averages can be calculated in the phase space formulation of quantum mechanics using the Wigner function in the usual way of a density function, so classical averages can be calculated in the Hilbert space formulation of classical mechanics using the Groenewold operator in the usual way of a density operator. Finally, just as the Wigner function evolves in time in accordance with a deformation of classical mechanical evolution, governed by a deformed Poisson bracket (the star or Moyal bracket), so the Groenewold operator evolves according to a deformation of quantum mechanical evolution, governed by a deformed commutator bracket \[5\], which has been called elsewhere the odot bracket \[9\].

The time evolution of Groenewold operators in Hilbert space can also be described using a superoperator formalism that is particularly convenient for numerical work, as shown by Muga et. al. \[7, 8\]. More recently \[9\], an expression has been derived for the classical evolution on Hilbert space as a series in increasing powers of \(\hbar\) with the quantum evolution as leading term. This form of the evolution suggests the possibility of probing the classical/quantum interface from the quantum side, by calculating classical corrections to a quantum evolution, rather than quantum corrections to a classical evolution.

It is desirable to understand the spectra of Groenewold quasi-density operators because of their primary role as the Hilbert space representatives of classical states. Some insight into how negative eigenvalues of Groenewold operators can arise is provided by the recent observation \[15\] that if a nonlinear classical evolution is applied to an initial quantum density operator corresponding to a coherent state (such an operator is also a non-negative definite Groenewold operator, corresponding to a Gaussian initial density on phase space), then the evolved operator develops negative eigenvalues. This is a special case of a result obtained earlier \[7\] for initial density operators corresponding to more general pure states. With regard to characterising those Groenewold operators that are non-negative definite, we note that every non-negative Wigner function can also be regarded as a Liouville density, and the corresponding true density operator is therefore also a Groenewold operator that is non-negative definite. However, the problem of identifying all non-negative Wigner functions has been solved only partially \[12\]. The only pure states having non-negative Wigner functions are coherent states (modulo a linear canonical transformation), and all such Wigner functions are Gaussians. Although progress has been made in extending these results to mixed states \[13, 14\], the extent of the set of all non-negative mixed-state Wigner functions is still unknown.

In what follows, we are concerned with properties of Groenewold operators
at a fixed time, and not with their evolution. We consider a classical system with one linear degree of freedom, in the phase plane $\Gamma$ and in Hilbert space $\mathcal{H}$. We examine the eigenvalue spectra of Groenewold operators in $\mathcal{H}$ corresponding to (A) classical densities that are Gaussian on $\Gamma$ and (B) classical densities that are uniform on a circular or elliptical disk in $\Gamma$, and zero elsewhere. In both cases the eigenvalues can be calculated exactly. In Case (A), we show that negative eigenvalues, and eigenvalues that exceed 1, appear when the classical uncertainty product $\Delta q \Delta p$ falls below $\hbar/2$, the minimum allowed by quantum mechanics, and we discuss the limiting form of the spectrum as the Gaussian approaches a delta-function.

The reader might be misled into thinking that a general classical density will give rise to a positive Groenewold operator whenever the uncertainty product is greater than $\hbar/2$. This is not so, and we show that in Case (B) the corresponding Groenewold operators have negative eigenvalues for all values of $\Delta q \Delta p$.

## 2 Groenewold quasi-density operators

We denote a general classical (Liouville) density on $\Gamma$ by $\rho(q, p)$. It satisfies

$$\rho(q, p) \geq 0, \quad \int_{\Gamma} \rho(q, p) = 1. \quad (1)$$

The corresponding Groenewold operator may be defined through the inverse Weyl-Wigner transform:

$$\hat{\rho} = 2\pi \hbar \mathcal{W}^{-1}(\rho) = \int_{\Gamma} \rho(q, p) \hat{\Delta}(q, p) dq dp, \quad (2)$$

where $\hat{\Delta}(q, p)$ is the Weyl-Wigner kernel \[16\], which may be defined as \[17\]

$$\hat{\Delta}(q, p) = 2 \mathcal{D}(q, p) \hat{P} \mathcal{D}(q, p)^\dagger = 2 \hat{\Delta}(2q, 2p) \hat{P}. \quad (3)$$

Here $\hat{P}$ denotes the parity operator and $\hat{D}(q, p) = \exp(i(q\hat{p} - p\hat{q})/\hbar)$ is a unitary displacement operator. Note that the eigenvalues of $\hat{\Delta}(q, p)$ are $\pm 2$ \[18\] and since Groenewold operators can be expressed as a convex combination of these operators as in \[2\] their eigenvalues lie in the range $[-2, 2]$, whereas those for a true density operator are restricted to the interval $[0, 1]$.

If $A(q, p), \ B(q, p)$ are classical functions on phase space and $\hat{A} = \mathcal{W}^{-1}(A), \ \hat{B} = \mathcal{W}^{-1}(B)$ are their operator images under the inverse Weyl-Wigner transform, then we have \[19\]

$$\frac{1}{2\pi \hbar} \int_{\Gamma} A(q, p) dq dp = \text{Tr}(\hat{A}), \quad \frac{1}{2\pi \hbar} \int_{\Gamma} A(q, p) B(q, p) dq dp = \text{Tr}(\hat{A}\hat{B}). \quad (4)$$

Note also that if $A(q, p)$ is real-valued, $\hat{A}$ is Hermitian. These properties ensure that a Groenewold operator $\hat{\rho} = \mathcal{W}^{-1}(\rho)$ has a number of important features
in common with true density operators: it is an Hermitian operator with unit trace \[9\] and the trace of the product of two Groenewold operators satisfies

\[
\text{Tr}(\hat{\rho}\hat{\rho}') = 2\pi \hbar \int \rho(q,p)\rho'(q,p)dqdp \geq 0 .
\] (5)

Furthermore, as mentioned above, the calculation of classical averages on Hilbert space takes the familiar form used for quantum averages, with the Groenewold operator acting in the role of a density operator:

\[
\langle A \rangle = \int \rho(q,p)A(q,p)dqdp = \text{Tr}(\hat{\rho}A) .
\] (6)

3 Gaussian densities

Despite the similarities between Groenewold operators and true density operators, there are important differences, the most obvious of which is the failure of the Groenewold operator to be non-negative definite in general.

The uncertainty product \(\Delta q\Delta p\) associated with a classical density is non-negative but can be arbitrarily small, and it is not surprising to find signatures of ‘non-quantum’ behaviour in the Hilbert space representation of classical densities appearing when this uncertainty product is less than \(\hbar/2\), the minimum value allowed in quantum mechanics.

In order to investigate this further, we introduce the class of Gaussian densities

\[
\rho_{\beta,\gamma}^{(G)}(q,p) = \frac{1}{\pi\beta\gamma} e^{-\left(q^2/\beta^2 + p^2/\gamma^2\right)} ,
\] (7)

where \(\beta, \gamma\) are constants with units of Length and Momentum respectively. The corresponding classical uncertainty is given by \(\Delta q\Delta p = \beta\gamma/2\).

From (2) we see that the corresponding Groenewold operators are given by

\[
\hat{\rho}_{\beta,\gamma}^{(G)} = \int \rho_{\beta,\gamma}^{(G)}(q,p)\hat{\Delta}(q,p)d\Gamma .
\] (8)

We now introduce the complex-conjugate variables \(\alpha, \bar{\alpha}\) with \(\alpha = (\sqrt{\gamma/\beta} q + i\sqrt{\beta/\gamma} p)/\sqrt{2\hbar}\) and the corresponding annihilation-creation operator pair \(\hat{a}, \hat{a}^\dagger\) with \(\hat{a} = (\sqrt{\gamma/\beta} q + i\sqrt{\beta/\gamma} p)/\sqrt{2\hbar}\), together with the “number operator” \(\hat{N} = \hat{a}^\dagger\hat{a}\). This allows us to define the Fock basis

\[
\{ |n\rangle, n = 0, 1, 2, \ldots \} , \quad \hat{a}|0\rangle = 0 , \quad |n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle , \quad \hat{N}|n\rangle = n|n\rangle .
\] (9)

The reason for introducing this basis is that the Groenewold operators \(\hat{\rho}_{\beta,\gamma}^{(G)}\) commute with \(\hat{N}\) and are diagonal on the Fock states. This can be seen by a direct calculation of their matrix elements:

\[
\langle n|\hat{\rho}_{\beta,\gamma}^{(G)}|m\rangle = \langle m|\hat{\rho}_{\beta,\gamma}^{(G)}|n\rangle = \int \rho_{\beta,\gamma}^{(G)}(q,p)\hat{\Delta}(q,p)|n\rangle d\Gamma,
\] (10)
where, in terms of the variables $\alpha, \overline{\alpha}$, $\langle n|\hat{\Delta}(\alpha, \overline{\alpha})|m\rangle$ is given by \[18\]
\[9\]
\[10\]
\[11\]
If we introduce the polar-type variables $(t, \phi)$ with $\alpha = \sqrt{t/2}\exp(i\phi)$ and $\overline{\alpha} = \sqrt{t/2}\exp(-i\phi)$, then we may express \[13\] as
\[12\]
Except in the case that $n = m$, the integral over $\phi$ vanishes, and hence, $\hat{\rho}^{(G)}_{\beta, \gamma}$ is diagonal on the Fock states, with eigenvalues
\[13\]
Note that this result generalises in the sense that if $\hat{f} = \mathcal{W}^{-1}(f)$, where $f(q, p) = f(q^2/\beta^2 + p^2/\gamma^2)$, then $[\hat{f}, \hat{N}] = 0$ and the eigenvalues of $\hat{f}$ satisfy a formula that generalises \[13\].

After evaluating \[13\], we get the eigenvalues of $\hat{\rho}^{(G)}_{\beta, \gamma}$ in the simple form
\[14\]
Since $\Delta q \Delta p = \beta \gamma/2$ and no quantum state exists in which $\Delta q \Delta p < h/2$, one expects that non-quantum features of $\hat{\rho}^{(G)}_{\beta, \gamma}$ should be observed for $\beta \gamma < h$. The result \[14\] shows that this is indeed the case, since for $\beta \gamma < h$ and $n$ odd, the eigenvalue $\lambda_n^{(G)}(\beta, \gamma) < 0$, while at least one of the eigenvalues lies above 1. Hence for $\beta \gamma < h$, when the classical density $\rho^{(G)}_{\beta, \gamma}(q, p)$ may be called “strongly classical”, the Groenewold operator $\hat{\rho}^{(G)}_{\beta, \gamma}$ displays the non-quantum feature of negative eigenvalues and eigenvalues that exceed 1. This is analogous to the negative values exhibited by Wigner functions corresponding to “strongly quantum states”, such as excited Fock states \[20\].

When the operator $\hat{\rho}^{(G)}_{\beta, \gamma}$ is considered on the coordinate representation of Hilbert space, it appears as an integral operator with kernel \[11\]
\[15\]
Because the $\lambda_n^{(G)}(\beta, \gamma)$ are the eigenvalues of $\hat{\rho}^{(G)}_{\beta, \gamma}$, it follows that
\[16\]
where $\varphi_n(x)$ is the coordinate representative of the state $|n\rangle$. This has the well-known form of an oscillator eigenfunction,

$$
\varphi_n(x) = \text{const.} H_n(x\sqrt{\gamma/\beta\hbar}) e^{-\gamma x^2/(2\beta\hbar)},
$$

(17)

where $H_n$ is the Hermite polynomial [23], and then (15) and (16) give

$$
\int_{-\infty}^{\infty} e^{-(\beta\gamma+b)(\beta\gamma-h)x-(\beta\gamma+b)y^2/(4\beta^2\hbar^2)} H_n(y\sqrt{\gamma/\beta\hbar}) dy = \beta \sqrt{\pi} \lambda_n^{(G)}(\beta, \gamma) H_n(x\sqrt{\gamma/\beta\hbar}).
$$

(18)

This is a known identity [20] and provides a check on the validity of (14).

The spectral bounds on $\hat{\rho}_{\beta,\gamma}^{(G)}$ are graphed in fig. 1 against the classical uncertainty $\Delta q \Delta p$ (in units of $\hbar$). When $\Delta q \Delta p < \hbar/2$, we obtain the strongly classical Groenewold operators discussed above. At the point $\Delta q \Delta p = \hbar/2$, the Groenewold operator has only one non-zero eigenvalue $\lambda_0 = 1$, and is precisely the pure state density $|0\rangle\langle 0|$. For $\Delta q \Delta p$ above this critical value, the spectrum is uniformly positive and bounded by $\lambda_0 = 2\hbar/(2\hbar + \beta\gamma) < 1$ above. As such, for $\beta\gamma > \hbar$, the Groenewold operator $\hat{\rho}_{\beta,\gamma}^{(G)}$ may be considered as the mixed state quantum density

$$
\hat{\rho}_{\beta,\gamma}^{(G)} = \sum_{n=0}^{\infty} p_n |n\rangle\langle n|, \quad p_n \equiv \lambda_n^{(G)}(\beta, \gamma) > 0, \quad \sum_{n=0}^{\infty} p_n = 1.
$$

(19)

## 4 Uniform Densities

In the Gaussian Case (A) above, there seems to be an obvious connection between the value of the uncertainty product associated with the Liouville density and the appearance of negative eigenvalues of the corresponding Groenewold operator. This is not necessarily the case for more general densities, however, and we illustrate this point by considering Case (B), the family of uniformly distributed Liouville densities, defined on the interior of an ellipse in $\Gamma$, centred at the origin:

$$
\rho^{(U)}_{\beta,\gamma}(q, p) = \begin{cases} 
\frac{1}{\pi\beta\gamma}, & 0 \leq \frac{q^2}{\beta^2} + \frac{p^2}{\gamma^2} \leq 1, \\
0, & \text{otherwise}.
\end{cases}
$$

(20)

The uncertainty product associated with $\rho^{(U)}_{\beta,\gamma}(q, p)$ is $\Delta q \Delta p = \beta\gamma/4$.

The corresponding Groenewold operators are given by

$$
\hat{\rho}^{(U)}_{\beta,\gamma} = \int_{\Gamma} \rho^{(U)}_{\beta,\gamma}(q, p) \hat{\Delta}(q, p) dq dp.
$$

(21)

We recognise these as scaled versions of operators that have been considered previously in a different context [22]. They also commute with $\hat{N}$ as defined above and their eigenvalues may be expressed as

$$
\lambda_n^{(U)}(\beta, \gamma) = \frac{2(-1)^n}{\beta\gamma} \int_0^{\beta\gamma} e^{-t} L_n(2t) dt, \quad n = 0, 1, 2, \ldots.
$$

(22)
Figure 1: Spectral bounds on $\hat{\rho}^{(G)}_{\beta,\gamma}$ (left) and $\hat{\rho}^{(U)}_{\beta,\gamma}$ (right). Note that when the classical uncertainty product exceeds $\hbar/2$, the Groenewold operators for the Gaussians considered in Case (A) are non-negative definite. On the right we show that no such transition occurs for the Groenewold operators corresponding to the uniform distributions considered in Case (B).

In fig. 1 the bounds on the spectrum of $\hat{\rho}^{(U)}_{\beta,\gamma}$ are graphed against $\beta\gamma$ (in units of $\hbar$), from which one sees that although the bounds decrease in magnitude as $\Delta q\Delta p$ rises above $\hbar/2$, the lower bound remains below zero.

There is a simple physical explanation for this phenomenon: by constructing a uniform distribution over a finite subregion of $\Gamma$, one is restricting both the position and momentum of a particle to a finite interval. This is impossible for a quantum system because the configuration and momentum space states are related by the Fourier transform and it is known that the Fourier transform of a function with compact support is entire $[24]$. This argument applies not only to Case (B) but to any Liouville density with compact support in $\Gamma$: for any such density, the corresponding Groenewold operator cannot be a true quantum density and it follows that since it has a trace equal to 1, it must have at least one negative eigenvalue in its spectrum. However, we note that for the example considered here, the negative values decrease in amplitude as the area of the ellipse increases.

5 Conclusion

Just as Wigner functions play a central role in the phase space formulation of quantum mechanics, so Groenewold operators play a central role in the Hilbert space formulation of classical mechanics, which offers the possibility of new insights into the classical-quantum interface. It is therefore important to elucidate the properties of Groenewold operators. In the present work, we have consid-
ered exactly solvable examples to illustrate some specific properties. We have seen that “violation of the uncertainty principle” and restriction to a compact subregion of $\Gamma$ can lead to eigenvalues outside of the range $[0,1]$, but this can occur due to the influence of other factors. The emergence of negative eigenvalues when Groenewold operators that are initially true density operators are allowed to evolve classically rather than quantum mechanically \cite{7,15} is a prime example. There is evidence \cite{15} to suggest that when the effects of the classical and quantum evolution diverge rapidly (such as for a delta-kicked rotator), the magnitude of the negative eigenvalues is much greater than for slowly diverging evolutions (such as for the Duffing oscillator). In recent work, we have shown that large negative eigenvalues arise in the classical evolution of an initial coherent state density \cite{25} in an anharmonic potential \cite{26} that causes the phase space density to develop “whorls”.

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